New class of RSO_2-NHC ligands and Pd/RSO_2-NHC complexes with tailored electronic properties and high performance in catalytic C-C and C-N bonds formation

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S1. General information and materials

General Procedures. Solvents were purified and dried according to standard methods and stored over activated 3 Å molecular sieves prior to use. Column chromatography was conducted on silica gel 60 (230−400 mesh, Merck). Glassware was dried at 120 °C in an oven for at least 3 h before use.

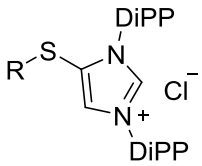
Instrumentation. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker Avance NEO 300 spectrometer at 300 MHz for ^{1}H and 75 MHz for ^{13}C in DMSO-d_6 or $CDCl_3$. The ^{1}H and ^{13}C NMR chemical shifts are reported relative to the solvent signals as internal standards: δ 2.50 (DMSO-d_6) or 7.26 ($CDCl_3$) for ^{1}H and δ 39.5 (DMSO-d_6) or 77.2 ($CDCl_3$) for ^{13}C.

High-resolution mass spectra (HRMS) were obtained on a Bruker maXis QTOF instrument (Bruker Daltonik GmbH, Bremen, Germany) equipped with an electrospray ionization (ESI) ion source. HRMS measurements were conducted in positive (+) MS ion mode (HV Capillary: 4500 V; Spray Shield: –500 V) with a scan range of *m/z* 50 – 1500. External calibration of the mass spectrometer was performed with the use of a low-concentration tuning mix solution, Agilent. Direct syringe injection was implemented for the analyzed solutions at a 3 μL min^{-1} flow rate. In HRMS measurements, nitrogen was applied as the nebulizer gas (0.4 bar) and dry gas (4.0 L min^{-1}). The dry temperature was 250 °C. All the spectra were recorded with 1 Hz frequency and processed using Bruker Data Analysis 4.0 software.

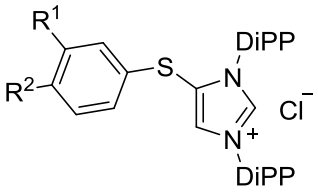
All geometry optimizations were performed by the PBE1PBE method[1, 2] using the def2-SVP basis set[3] in the Gaussian 09[4] software package. For further validation of the energetics and electronic properties of the ligands and palladium complexes, single-point calculations were performed on the PBE1PBE/Def2-SVP optimized geometries using hybrid GGA DFT functional PBE1PBE employing a valence triple-ζ-type basis set Def2-TZVP[5]. The solvent effects ($CHCl_3$, ε = 4.71) were evaluated implicitly by a self-consistent reaction field (SCRF) approach using the IEF PCM continuum solvation model[6, 7]. The convergence criteria were used as default, and the vibrational analysis was also carried out under standard conditions (1 atm., 298.15 K).

The percent buried volume $\%V_{bur}$ was obtained from topographic steric maps analysis of model palladium complexes using the SambVca 2.1 web tool[8] (parameters: sphere radius 3.50 Å; mesh spacing 0.05; bond radii scaled by 1.17; H atoms are excluded). The ETS-NOCV analysis was performed with the Multiwfn program[9]. The molecular structures and isosurfaces of frontier orbitals, ETS-NOCV pairs and MESP densities were visualized using Chemcraft[10] software.

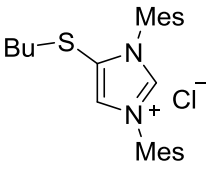
Materials. Compounds **1a-r** were synthesized as described in the literature.[11] All other chemicals were purchased from commercial sources.



1a, R = C_6H_5
1b, R = Bu



1c, R^1 = H, R^2 = Me
1d, R^1 = H, R^2 = Cl
1e, R^1 = R^2 = Cl



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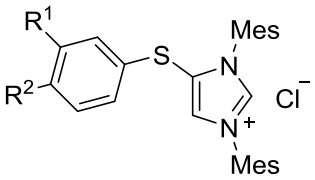
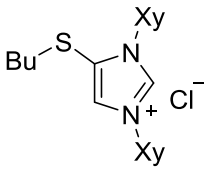
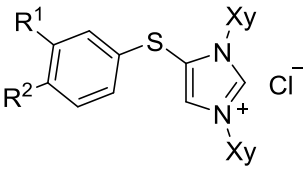


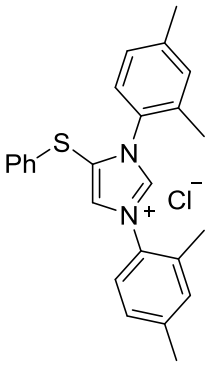
1g, R^1 = R^2 = H
1h, R^1 = H, R^2 = Me
1i, R^1 = H, R^2 = Cl
1j, R^1 = OCH_3, R^2 = H



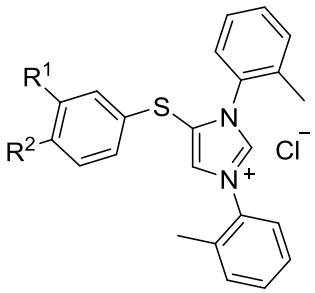
1k



1l, R^1 = R^2 = H
1m, R^1 = H, R^2 = Me
1n, R^1 = H, R^2 = Cl



1o



1p, R^1 = H, R^2 = Me
1q, R^1 = H, R^2 = Cl
1r, R^1 = OCH_3, R^2 = H

Figure S1. Structures of starting compounds **1a-r**.

S2. Extended DFT data

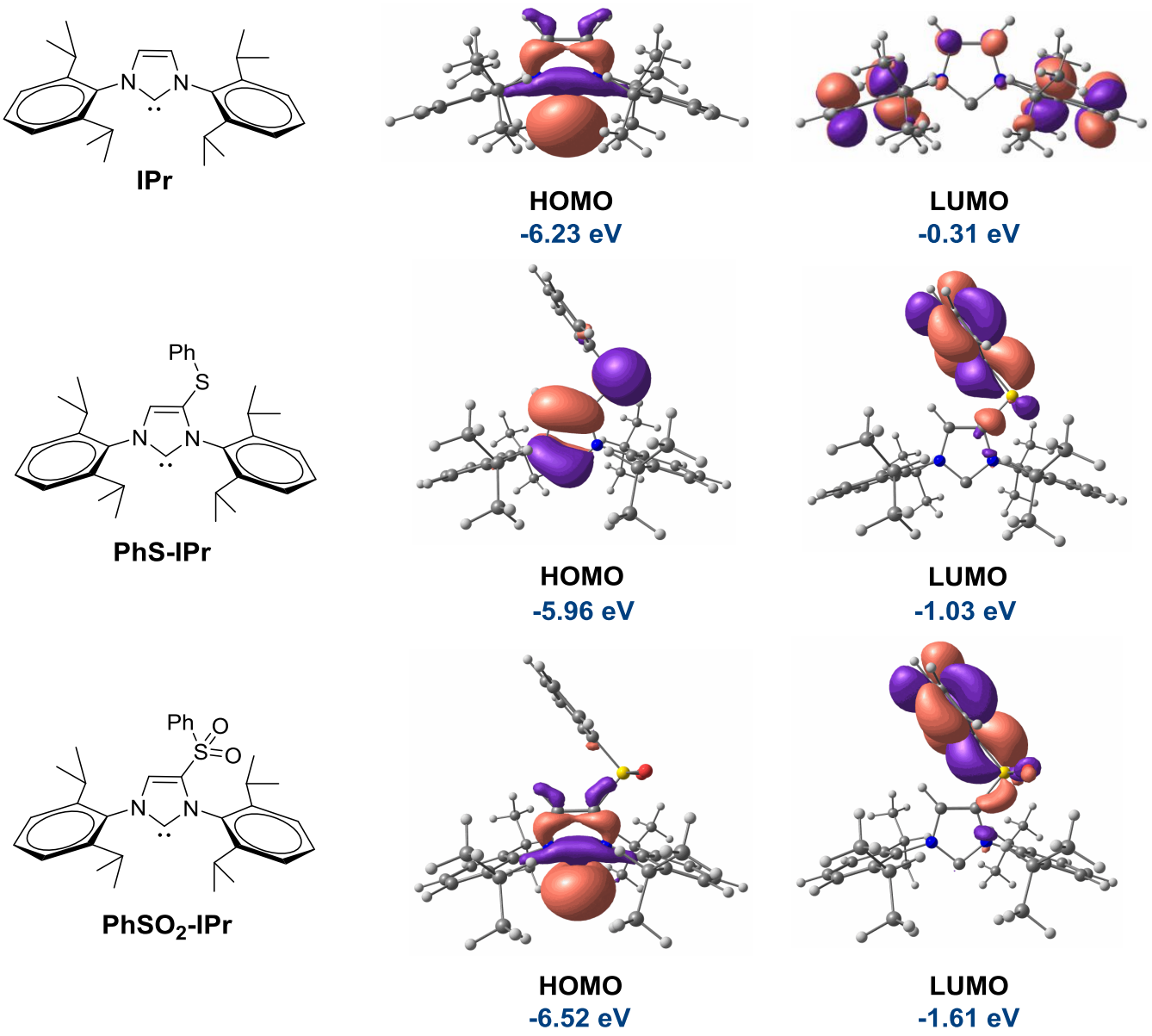


Figure S2. Plots and energy values (in eV) of the HOMO and LUMO calculated at PBE1PBE/def2tzvp//PBE1PBE/def2svp in $CHCl_3$ solution (IEF-PCM).

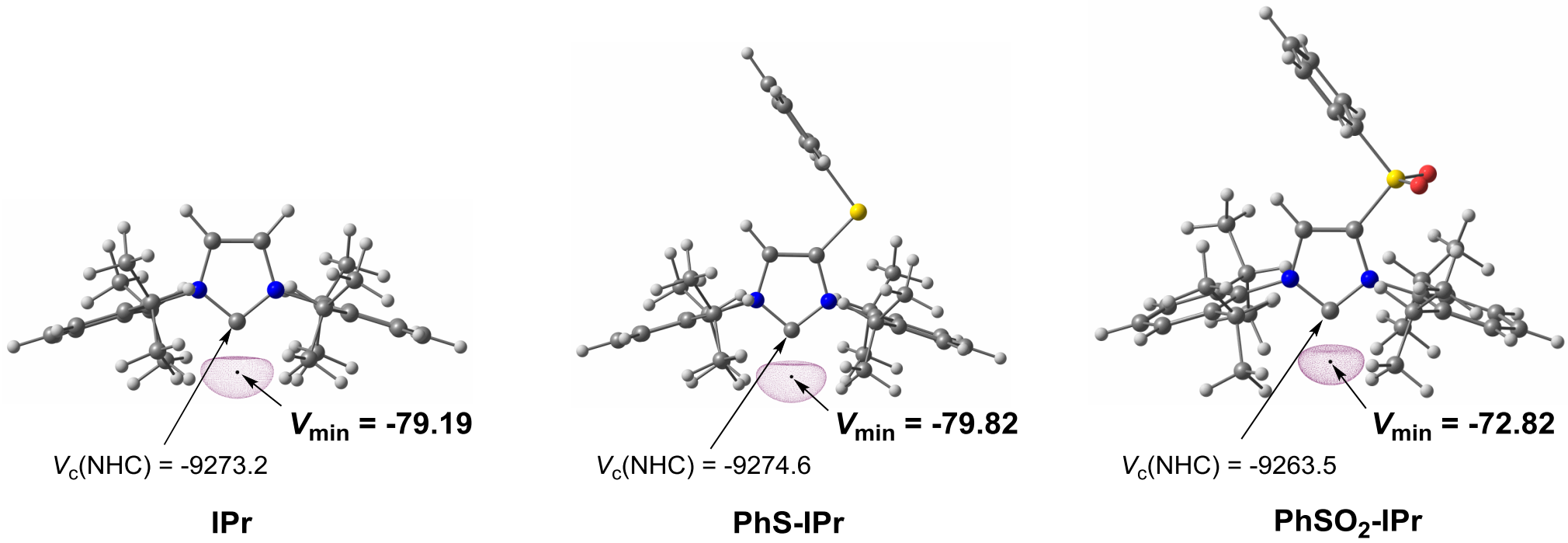
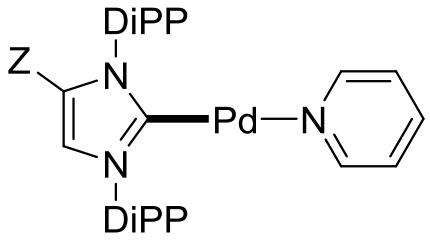


Figure S3. Molecular electrostatic potential isosurface at -50 kcal·mol^{-1} of model NHC-ligands calculated at PBE1PBE/def2tzvp//PBE1PBE/def2svp in $CHCl_3$ solution (IEF-PCM). The black dots represent the location of the V_{min} points. V_{min} and V_c values are given in kcal·mol^{-1}.



9a-c

Complex	BDE, kcal/mol
9a, Z = H	53.9
9b, Z = SPh	53.9
9c, Z = SO_2Ph	53.6

Figure S4. Pd-$C_{(NHC)}$ bond dissociation energy (BDE) calculated at PBE1PBE/def2tzvp//PBE1PBE/def2svp in molecules **9a-c**.

S3. Single crystal X-ray diffraction data

X-ray diffraction data for **(IPr)PdSPh** and **3a** were collected at 100 K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area detector (kappa geometry, shutterless ω-scan technique) using monochromatized Mo K_α-radiation. The intensity data were integrated and analytically corrected for absorption and decay by the CrysAlisPro program.[12] The structures were solved by direct methods using SHELXT[13] and refined by the full-matrix least-squares method on F^2 using SHELXL-2018[14] in the OLEX2 program.[15] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions (C-H distance = 0.950 Å for aromatic, 0.980 Å for methyl, 0.990 Å for methylene and 1.000 Å for tertiary hydrogen atoms) and refined as riding atoms with relative isotropic displacement parameters taken as U_{iso}(H)=1.5U_{eq}(C) for methyl groups and U_{iso}(H)=1.2U_{eq}(C) otherwise. The disordered fragments and molecules were modeled by applying similarity constraints on anisotropic displacement parameters on similar atoms and by constraining similar distances to be equal within the deviation of 0.003 Å.

Crystal data, data collection and structure refinement details for **3a** are summarized in Table S1. The structures have been deposited at the Cambridge Crystallographic Data Center with the reference CCDC numbers 2255010; they also contain the supplementary crystallographic data. These data can be obtained free of charge from the CCDC *via* https://www.ccdc.cam.ac.uk/structures/

Table S1. Crystal data, data collection and structure refinement details for **3a**

Identification code	**3a**
Empirical formula	$C_{39}H_{47}Cl_4N_3O_2PdS$
Formula weight	870.05
Temperature, K	100.0(2)
Wavelength, Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	
a, Å	11.69119(14)
b, Å	19.42369(17)
c, Å	18.9969(2)
β, °	107.4290(13)
Volume, $Å^3$	4115.87(8) $Å^3$
Z	4
Density (calculated), g/cm^3	1.404
Absorption coefficient (μ), mm^{-1}	0.797
F(000)	1792
Crystal size, mm	0.75×0.60×0.48
θ range for data collection, °	2.105-33.750
Index ranges	$-18 \le h \le 18$,
	$-29 \le k \le 30$,
	$-29 \le l \le 29$
Reflections	
Collected	97310
Independent [R_{int}]	16385 [0.0246]
Observed (I>2σ(I))	15026
Completeness to θ_{full} / θ_{max}	0.999 / 0.994
T_{max} / T_{min}	0.745 / 0.652
Data / restraints / parameters	16385 / 1013 / 774
Goodness-of-fit on F^2	1.075
R1/wR2 (I>2σ(I))	0.0286 / 0.0691
R1/wR2 (all data)	0.0323 / 0.0704
Extinction coefficient	0.00084(9)
$\Delta\rho_{min}$ / $\Delta\rho_{max}$, $ē \cdot Å^{-3}$	1.219 / -0.509
CCDC number	2255010

The structure of **3a.**

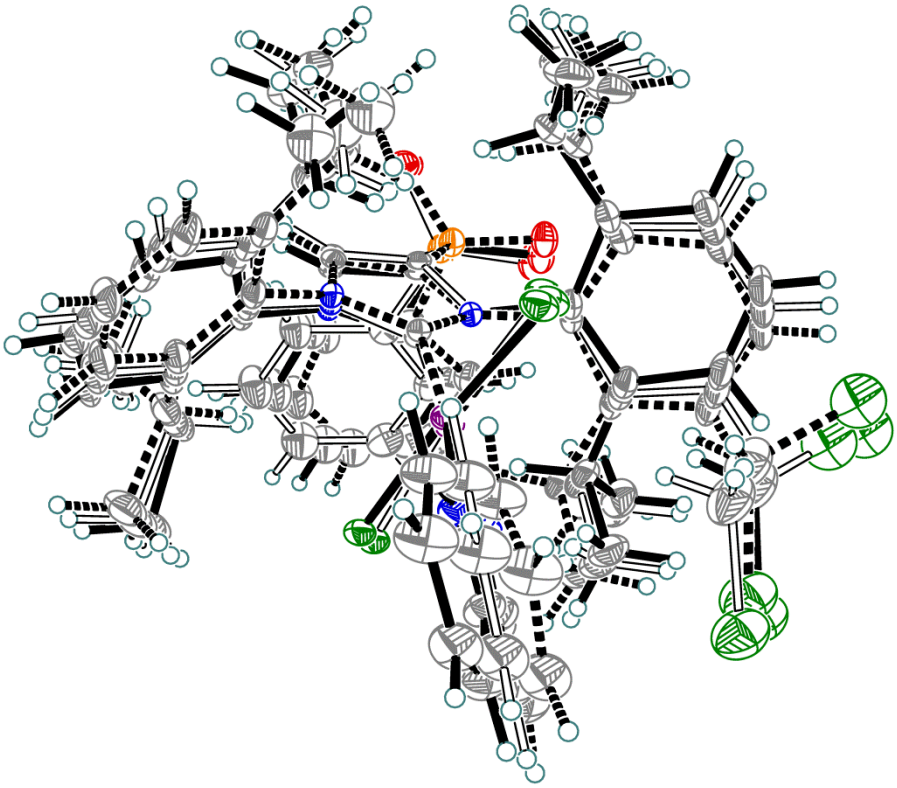


Figure S5. The structure of **3a** (p=50%). The molecule of the complex was modeled as disordered over three positions (the disorder ratio is 0.498(2):0.289(2):0.2132(19)). The lattice chloroform molecule is also disordered over three positions (0.845(3):0.070(2):0.085(3)).

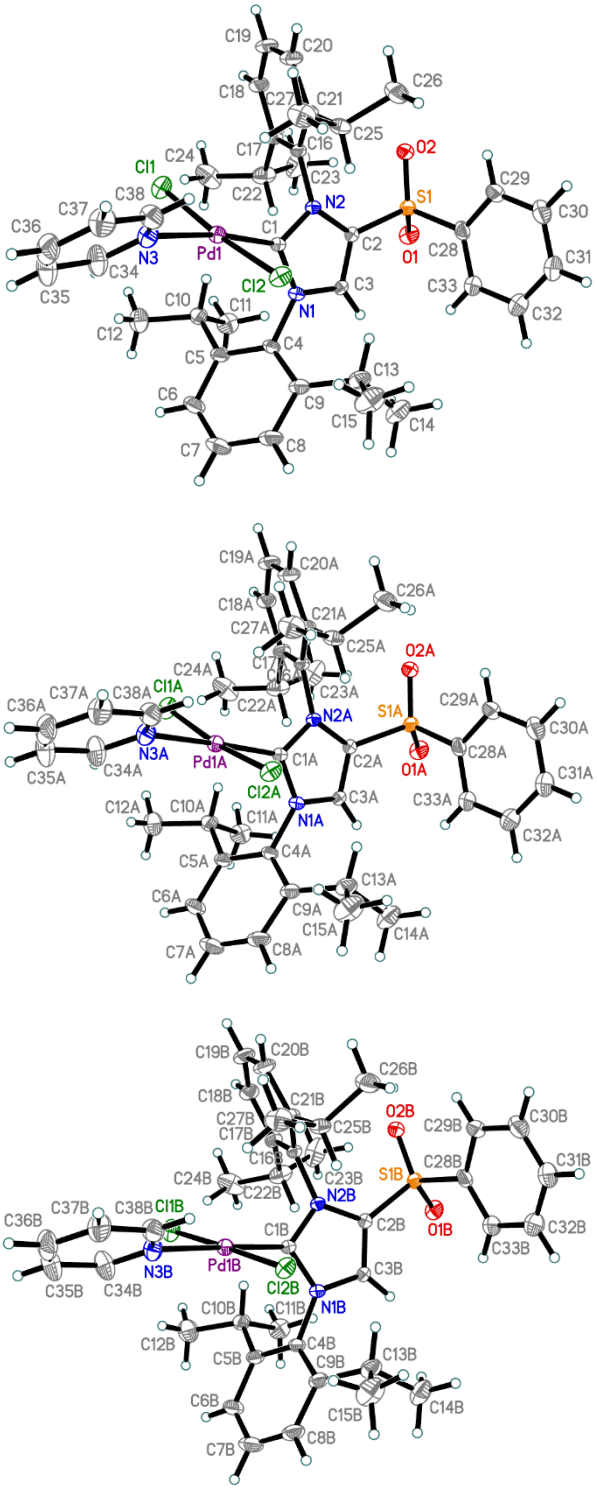


Figure S6. Three components for the disorder of molecule **3a** (p=50%) with atom site occupancies of 0.498(2) (top), 0.289(2) (middle) and 0.2132(19) (bottom).

Table S2. Selected bond distances in **3a**, in Å.

Pd1-Cl1	2.2975(14)	C5-C6	1.402(2)	C21-C25	1.512(2)
Pd1-Cl2	2.3032(14)	C5-C10	1.516(3)	C22-C23	1.532(2)
Pd1-C1	1.9678(17)	C6-C7	1.374(3)	C22-C24	1.530(2)
Pd1-N3	2.0974(18)	C7-C8	1.375(3)	C25-C26	1.533(2)
S1-O1	1.4415(18)	C8-C9	1.403(2)	C25-C27	1.530(2)
S1-O2	1.4323(17)	C9-C13	1.514(3)	C28-C29	1.390(2)
S1-C2	1.7591(18)	C10-C11	1.536(2)	C28-C33	1.390(2)
S1-C28	1.7664(19)	C10-C12	1.533(2)	C29-C30	1.394(3)
N1-C1	1.3647(19)	C13-C14	1.536(2)	C30-C31	1.376(3)
N1-C3	1.376(2)	C13-C15	1.533(2)	C31-C32	1.380(3)
N1-C4	1.449(2)	C16-C17	1.400(2)	C32-C33	1.392(2)
C1-N2	1.3582(19)	C16-C21	1.397(2)	N3-C34	1.341(2)
N2-C2	1.4016(19)	C17-C18	1.401(2)	N3-C38	1.340(2)
N2-C16	1.456(2)	C17-C22	1.511(2)	C34-C35	1.393(3)
C2-C3	1.353(2)	C18-C19	1.375(2)	C35-C36	1.379(3)
C4-C5	1.403(2)	C19-C20	1.374(2)	C36-C37	1.378(3)
C4-C9	1.400(2)	C20-C21	1.402(2)	C37-C38	1.392(2)
Pd1A-Cl1A	2.298(2)	C5A-C6A	1.402(3)	C21A-C25A	1.512(3)
Pd1A-Cl2A	2.304(2)	C5A-C10A	1.515(3)	C22A-C23A	1.532(2)
Pd1A-C1A	1.967(2)	C6A-C7A	1.373(3)	C22A-C24A	1.532(2)
Pd1A-N3A	2.097(2)	C7A-C8A	1.372(3)	C25A-C26A	1.532(2)
S1A-O1A	1.442(2)	C8A-C9A	1.403(3)	C25A-C27A	1.531(2)
S1A-O2A	1.432(2)	C9A-C13A	1.514(3)	C28A-C29A	1.390(3)
S1A-C2A	1.759(2)	C10A-C11A	1.535(2)	C28A-C33A	1.388(3)
S1A-C28A	1.766(2)	C10A-C12A	1.534(2)	C29A-C30A	1.394(3)
N1A-C1A	1.365(2)	C13A-C14A	1.536(2)	C30A-C31A	1.376(3)
N1A-C3A	1.376(2)	C13A-C15A	1.534(2)	C31A-C32A	1.376(3)
N1A-C4A	1.449(3)	C16A-C17A	1.400(2)	C32A-C33A	1.393(3)
C1A-N2A	1.358(2)	C16A-C21A	1.398(2)	N3A-C34A	1.341(3)
N2A-C2A	1.402(2)	C17A-C18A	1.402(2)	N3A-C38A	1.341(3)
N2A-C16A	1.456(2)	C17A-C22A	1.513(3)	C34A-C35A	1.392(3)
C2A-C3A	1.353(2)	C18A-C19A	1.375(3)	C35A-C36A	1.379(3)
C4A-C5A	1.403(2)	C19A-C20A	1.373(3)	C36A-C37A	1.379(3)
C4A-C9A	1.400(2)	C20A-C21A	1.403(2)	C37A-C38A	1.392(3)
Pd1B-Cl1B	2.299(2)	C5B-C6B	1.402(3)	C21B-C25B	1.510(3)
Pd1B-Cl2B	2.304(2)	C5B-C10B	1.512(3)	C22B-C23B	1.532(2)
Pd1B-C1B	1.967(2)	C6B-C7B	1.373(3)	C22B-C24B	1.531(2)
Pd1B-N3B	2.096(2)	C7B-C8B	1.373(3)	C25B-C26B	1.532(2)
S1B-O1B	1.442(2)	C8B-C9B	1.403(3)	C25B-C27B	1.531(2)
S1B-O2B	1.432(2)	C9B-C13B	1.514(3)	C28B-C29B	1.389(3)
S1B-C2B	1.759(2)	C10B-C11B	1.535(2)	C28B-C33B	1.388(3)
S1B-C28B	1.765(3)	C10B-C12B	1.534(2)	C29B-C30B	1.393(3)
N1B-C1B	1.365(3)	C13B-C14B	1.536(2)	C30B-C31B	1.377(3)
N1B-C3B	1.376(3)	C13B-C15B	1.536(2)	C31B-C32B	1.376(3)
N1B-C4B	1.450(3)	C16B-C17B	1.399(2)	C32B-C33B	1.393(3)
C1B-N2B	1.358(3)	C16B-C21B	1.398(2)	N3B-C34B	1.340(3)
N2B-C2B	1.401(3)	C17B-C18B	1.402(3)	N3B-C38B	1.338(3)
N2B-C16B	1.456(3)	C17B-C22B	1.511(3)	C34B-C35B	1.392(3)
C2B-C3B	1.354(3)	C18B-C19B	1.373(3)	C35B-C36B	1.379(3)
C4B-C5B	1.401(3)	C19B-C20B	1.372(3)	C36B-C37B	1.378(3)
C4B-C9B	1.401(3)	C20B-C21B	1.401(3)	C37B-C38B	1.391(3)

Table S3. Selected bond angles about the Pd atom in **3a**, °.

Cl1-Pd1-Cl2	174.4(4)	Cl1A-Pd1A-Cl2A	173.2(6)	Cl1B-Pd1B-Cl2B	178.1(5)
C1-Pd1-Cl1	95.2(3)	C1A-Pd1A-Cl1A	94.1(5)	C1B-Pd1B-Cl1B	90.5(5)
C1-Pd1-Cl2	85.2(3)	C1A-Pd1A-Cl2A	86.4(4)	C1B-Pd1B-Cl2B	88.3(5)
C1-Pd1-N3	172.2(3)	C1A-Pd1A-N3A	175.5(5)	C1B-Pd1B-N3B	178.6(4)
N3-Pd1-Cl1	89.1(2)	N3A-Pd1A-Cl1A	90.4(4)	N3B-Pd1B-Cl1B	89.1(3)
N3-Pd1-Cl2	91.16(18)	N3A-Pd1A-Cl2A	89.2(3)	N3B-Pd1B-Cl2B	92.1(3)

S4. ^{1}H and ^{13}C NMR spectra

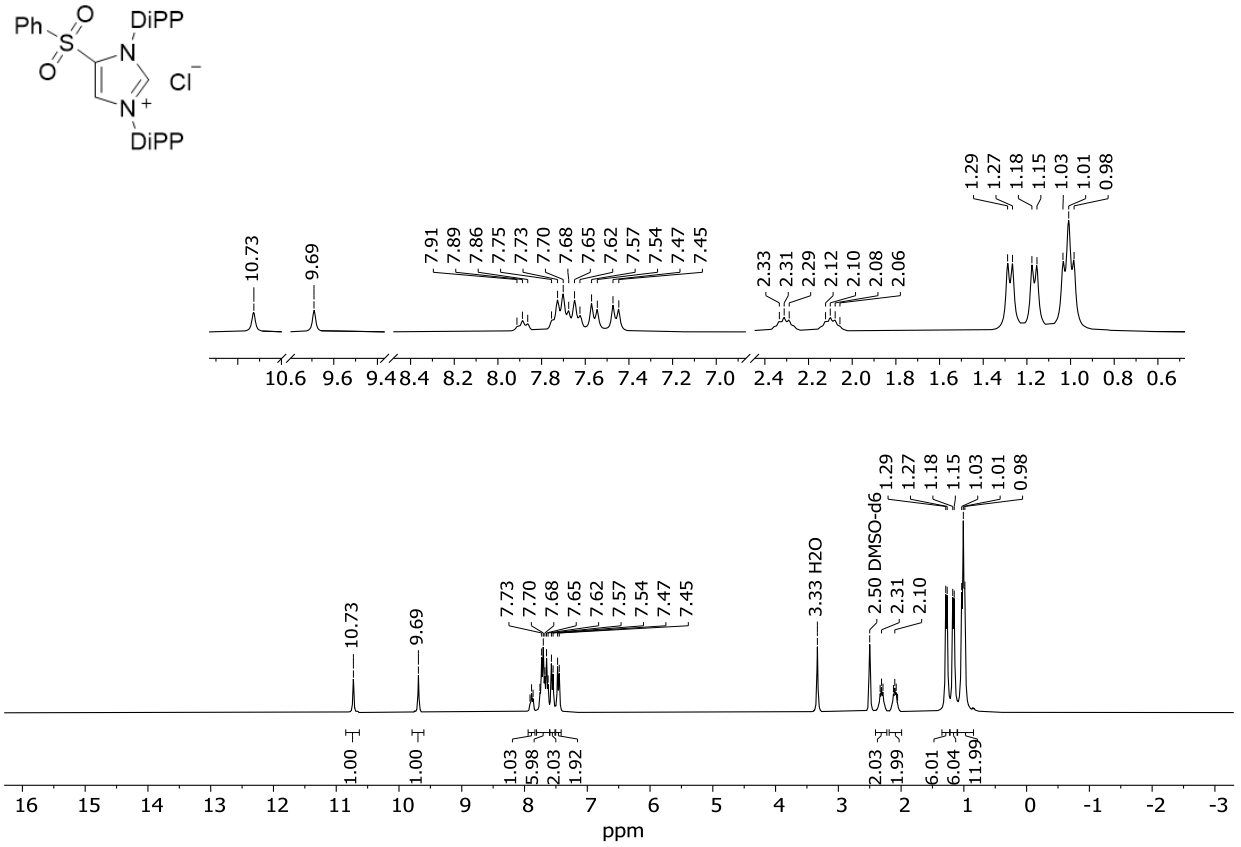


Figure S7. ^{1}H NMR spectrum of **2a** (DMSO-d_6, 300 MHz)

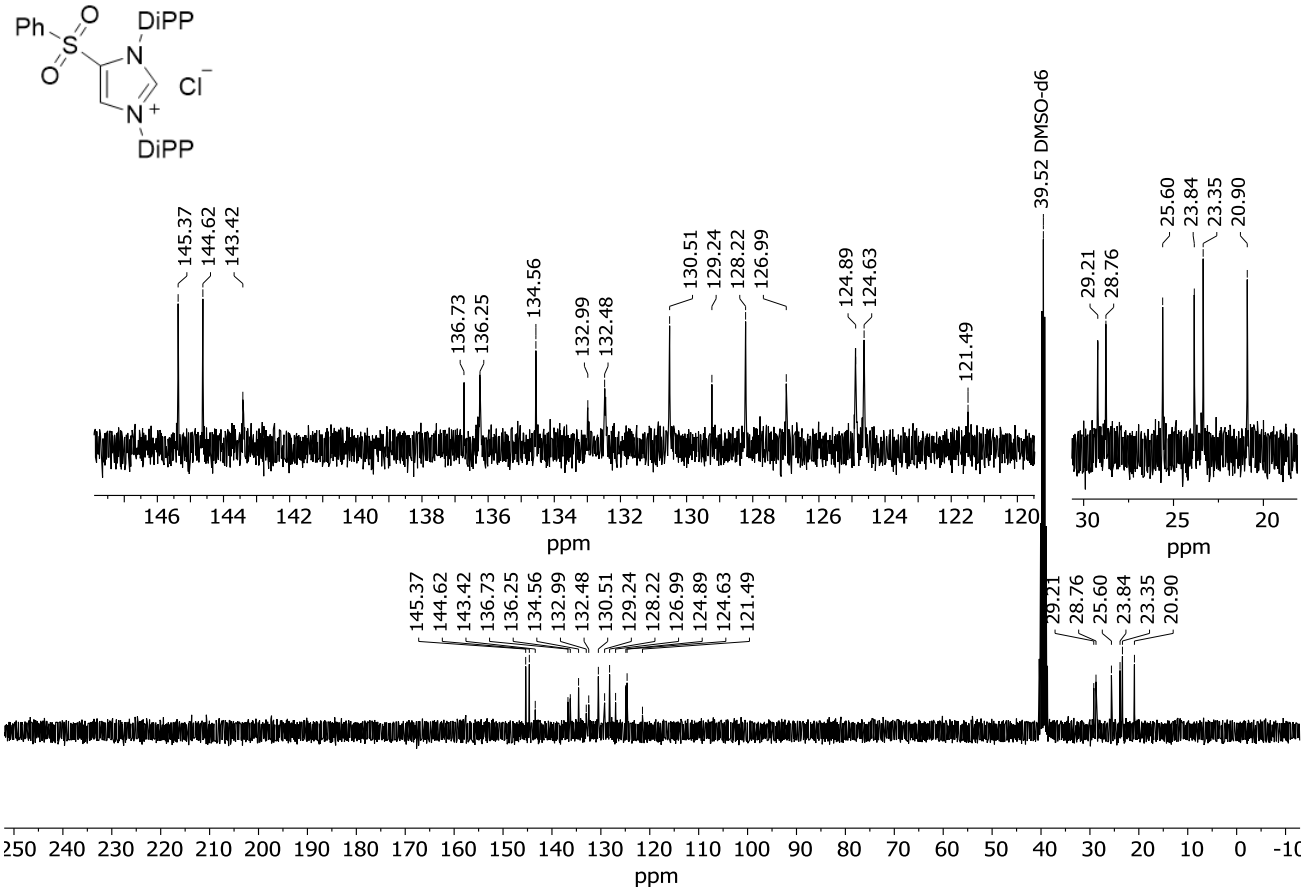


Figure S8. ^{13}C NMR spectrum of **2a** (DMSO-d_6, 75 MHz)

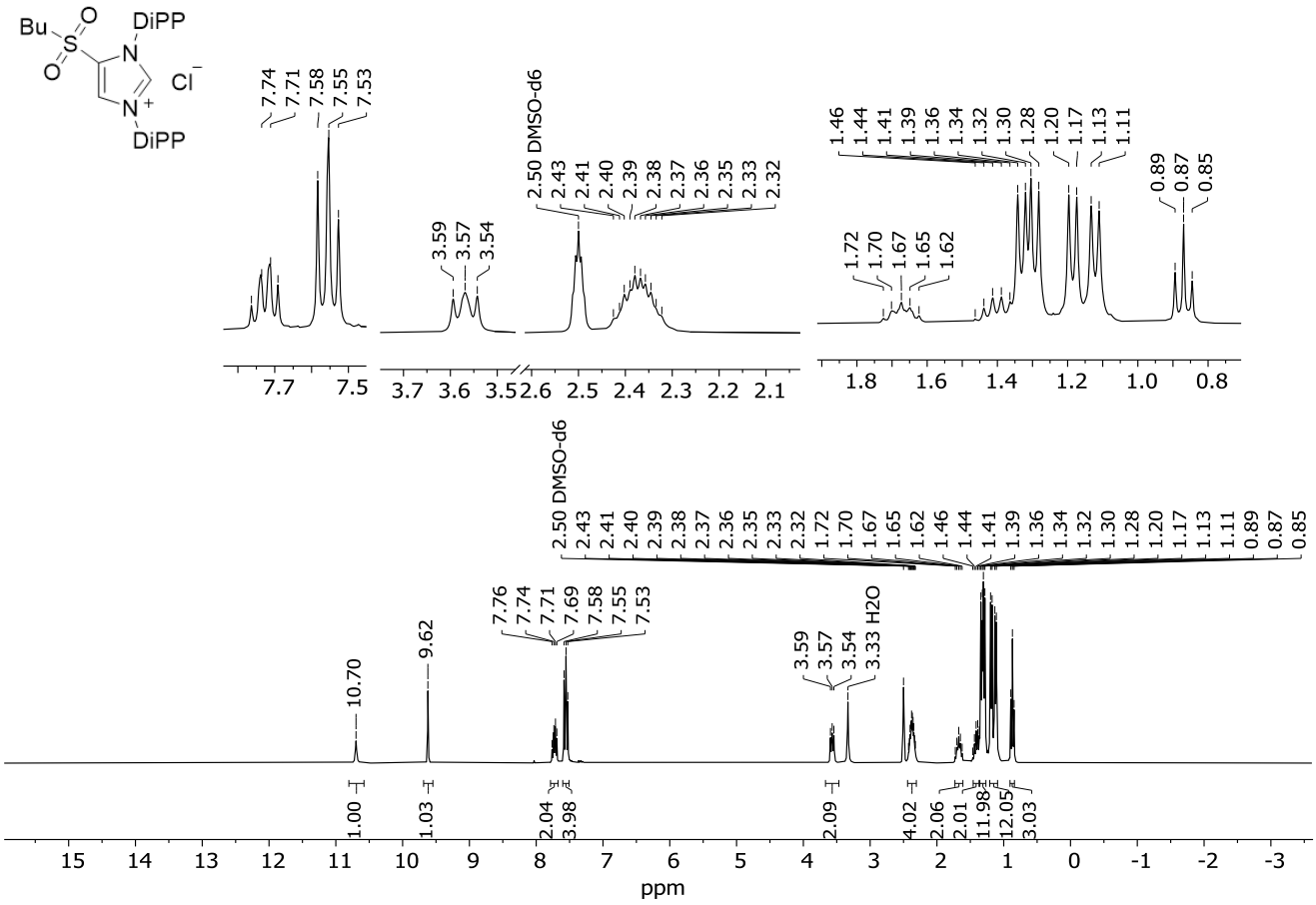


Figure S1. ^{1}H NMR spectrum of **2b** (DMSO-d_6, 300 MHz)

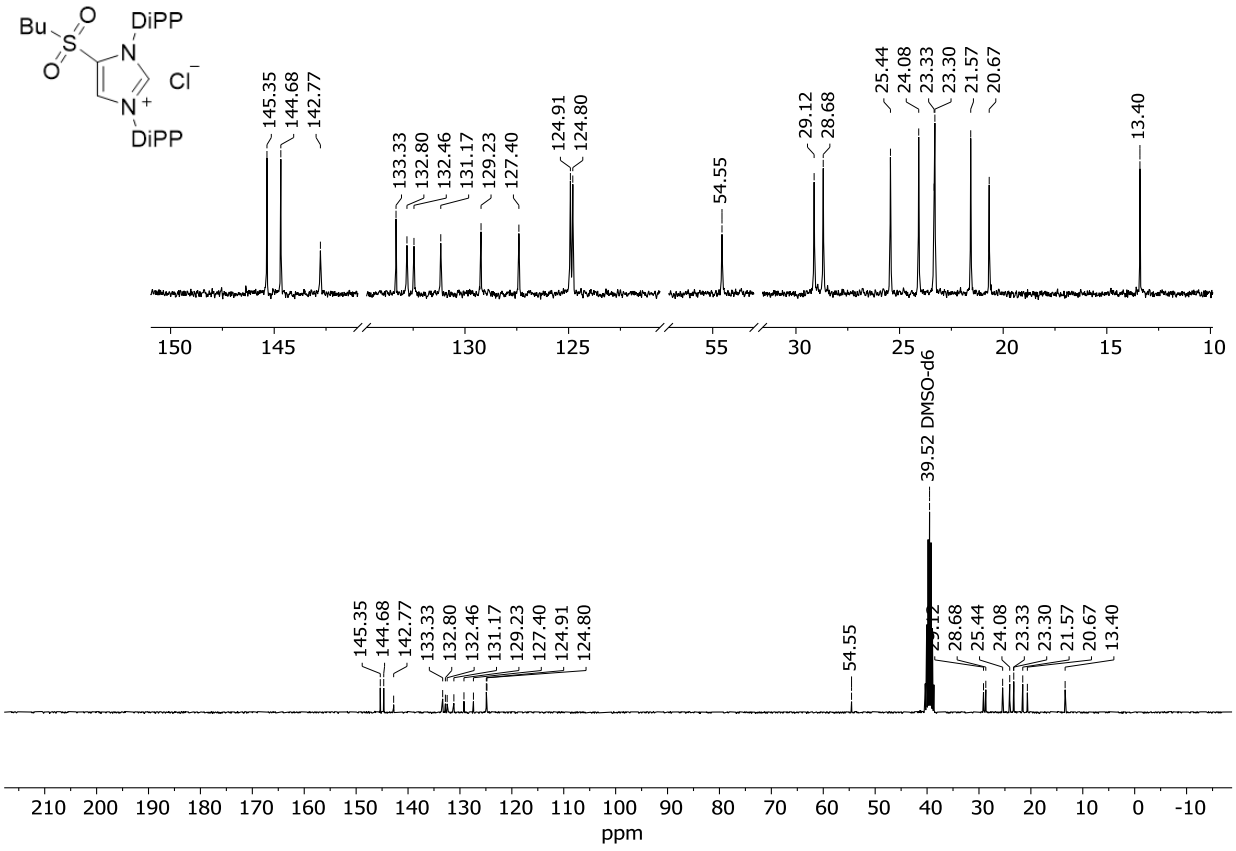


Figure S2. ^{13}C NMR spectrum of **2b** (DMSO-d_6, 75 MHz)

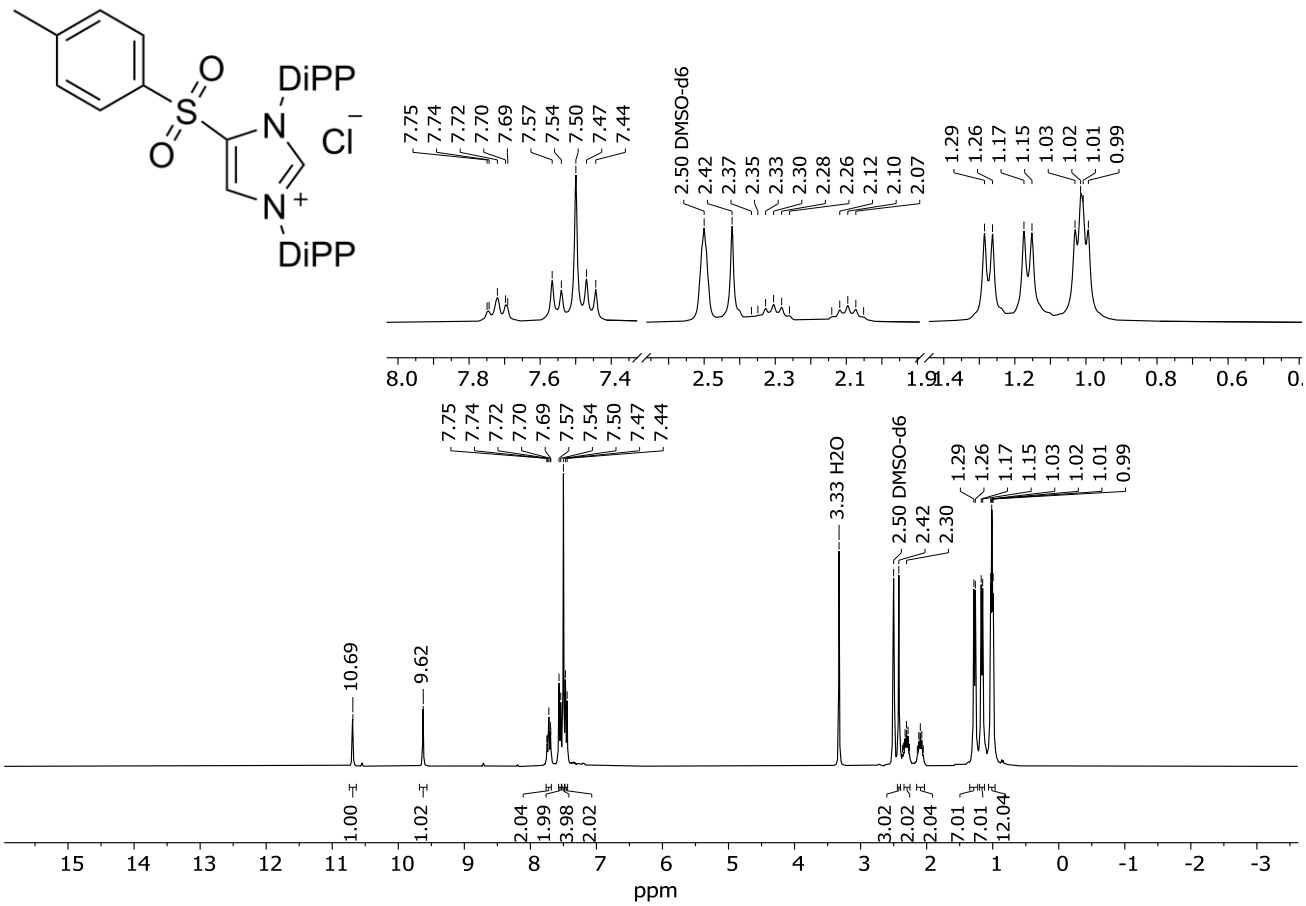


Figure S3. ^{1}H NMR spectrum of **2c** (DMSO-d_6, 300 MHz)

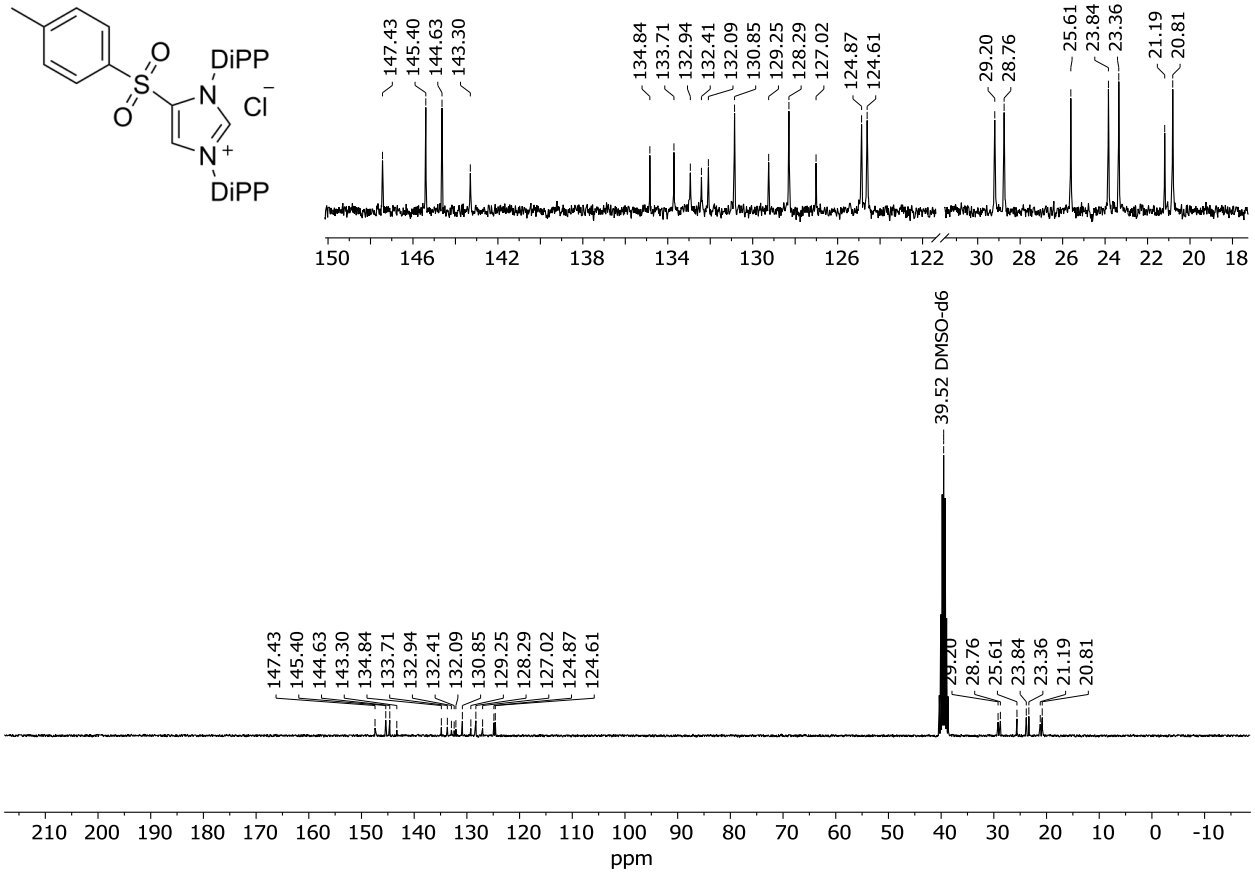


Figure S4. ^{13}C NMR spectrum of **2c** (DMSO-d_6, 75 MHz)

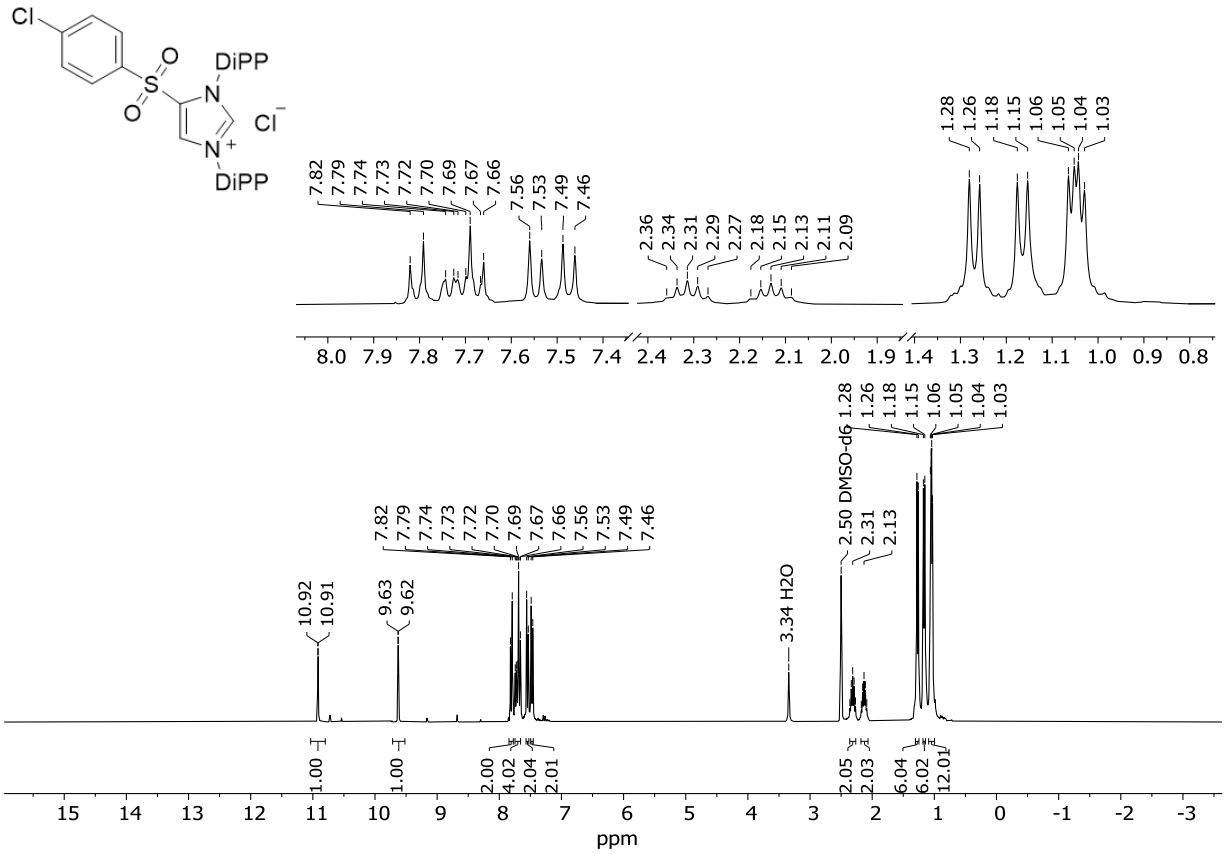


Figure S5. ^{1}H NMR spectrum of **2d** (DMSO-d_6, 300 MHz)

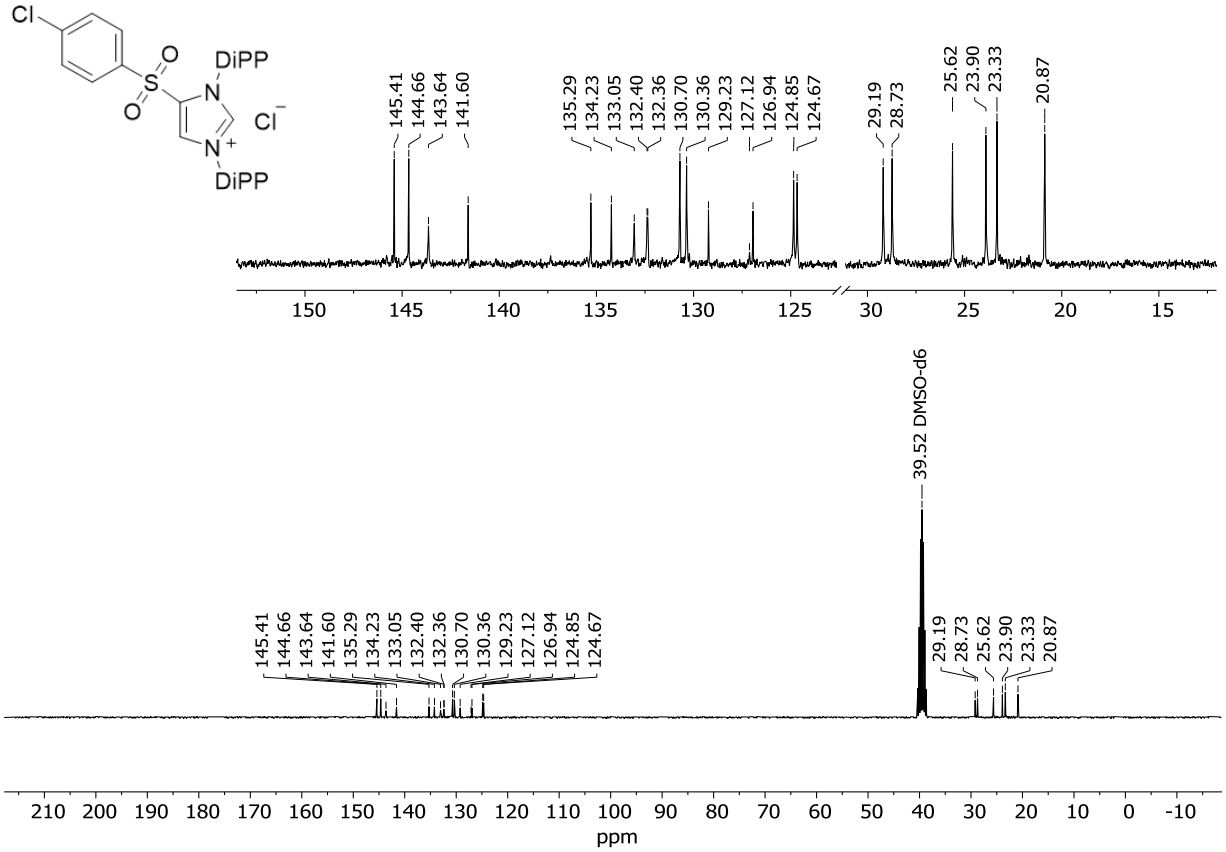


Figure S6. ^{13}C NMR spectrum of **2d** (DMSO-d_6, 75 MHz)

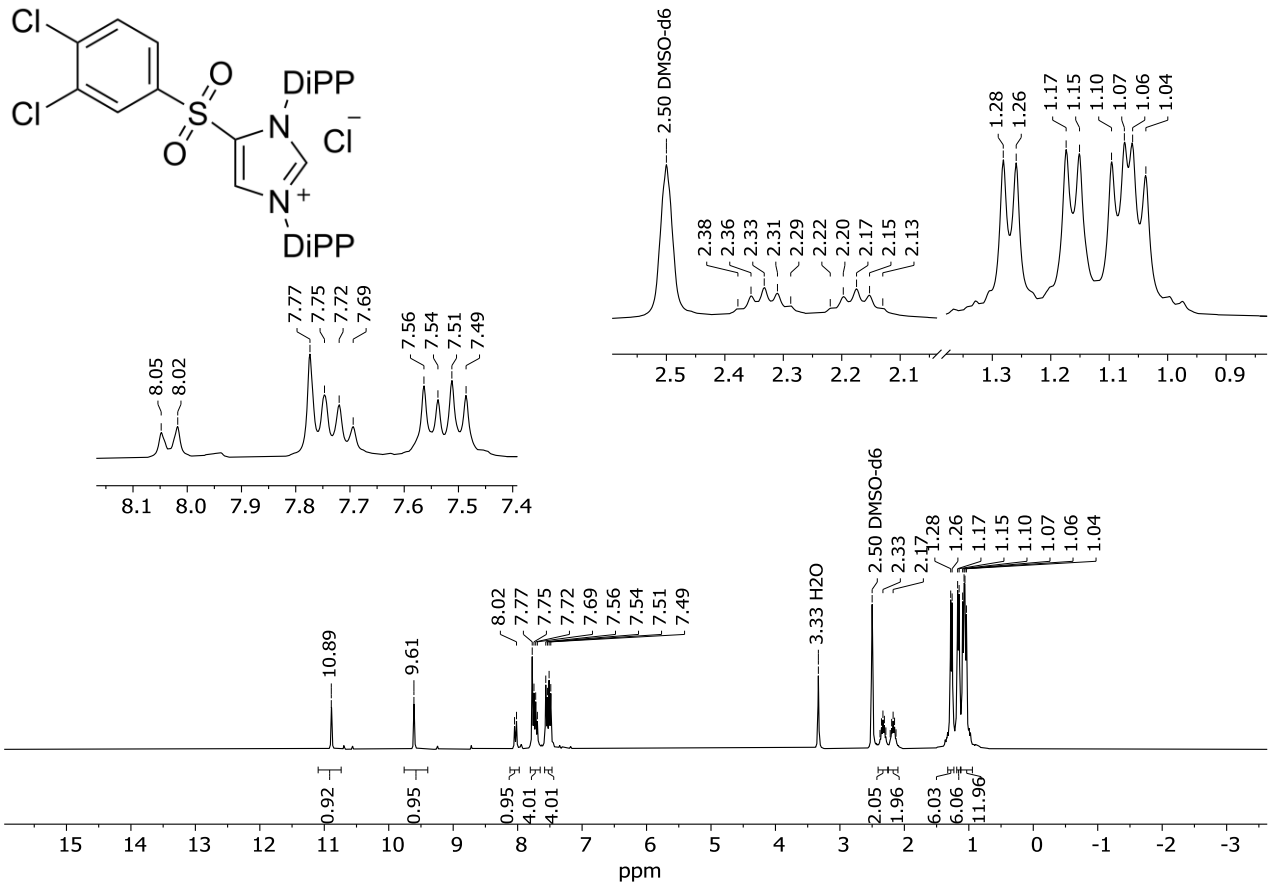


Figure S7.[1]H NMR spectrum of **2e** (DMSO-d_6, 300 MHz)

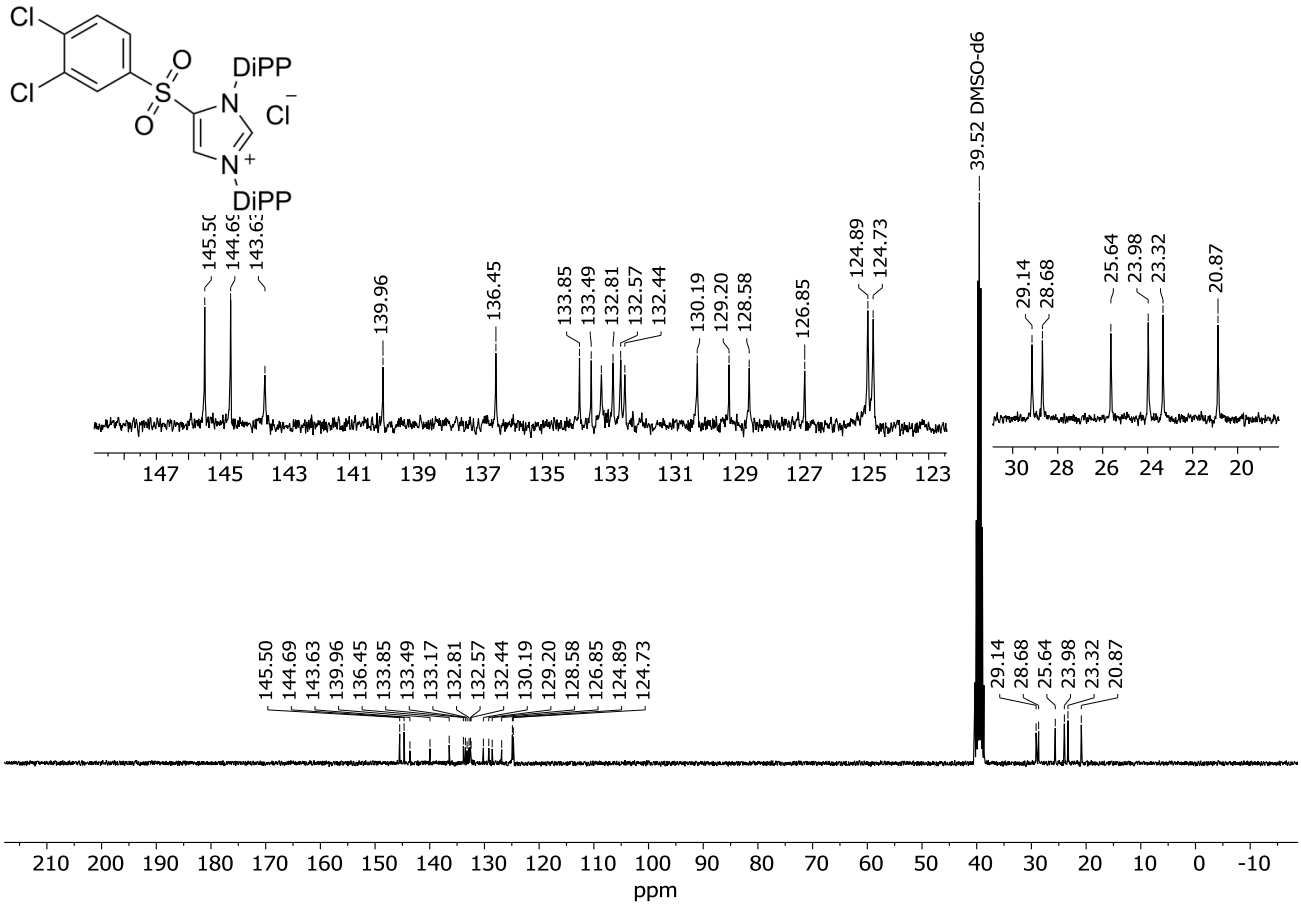


Figure S8.[13]C NMR spectrum of **2e** (DMSO-d_6, 75 MHz)

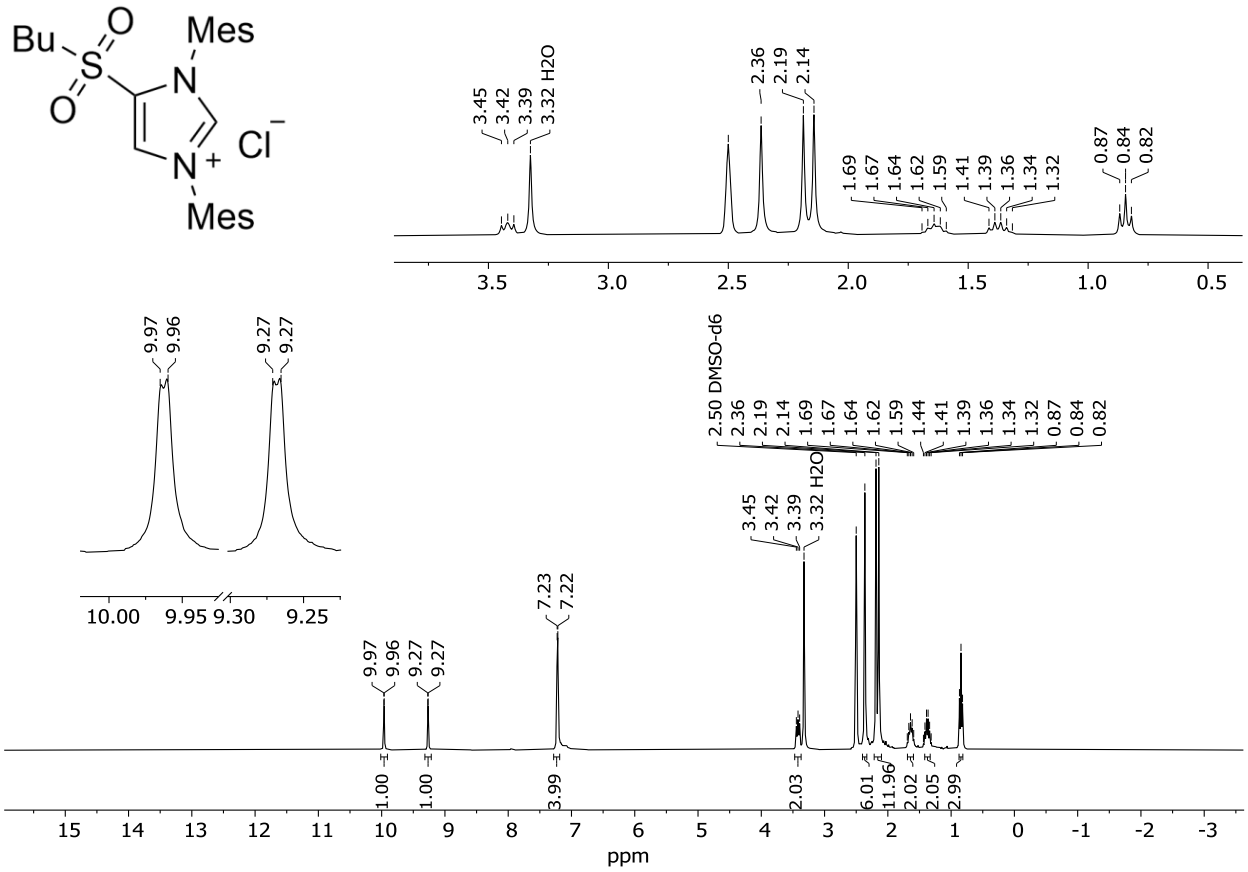


Figure S9. ^{1}H NMR spectrum of **2f** (DMSO-d_6, 300 MHz)

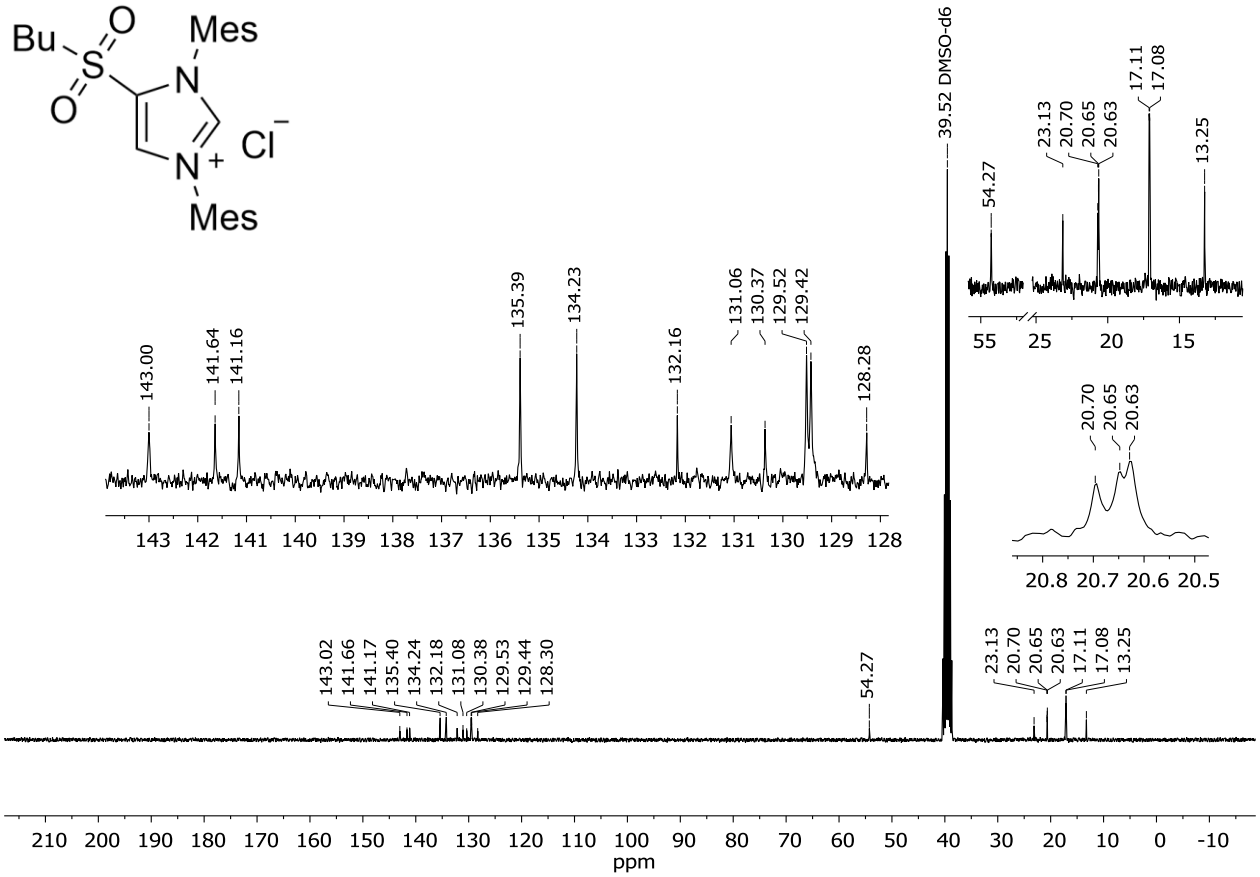


Figure S10. ^{13}C NMR spectrum of **2f** (DMSO-d_6, 75 MHz)

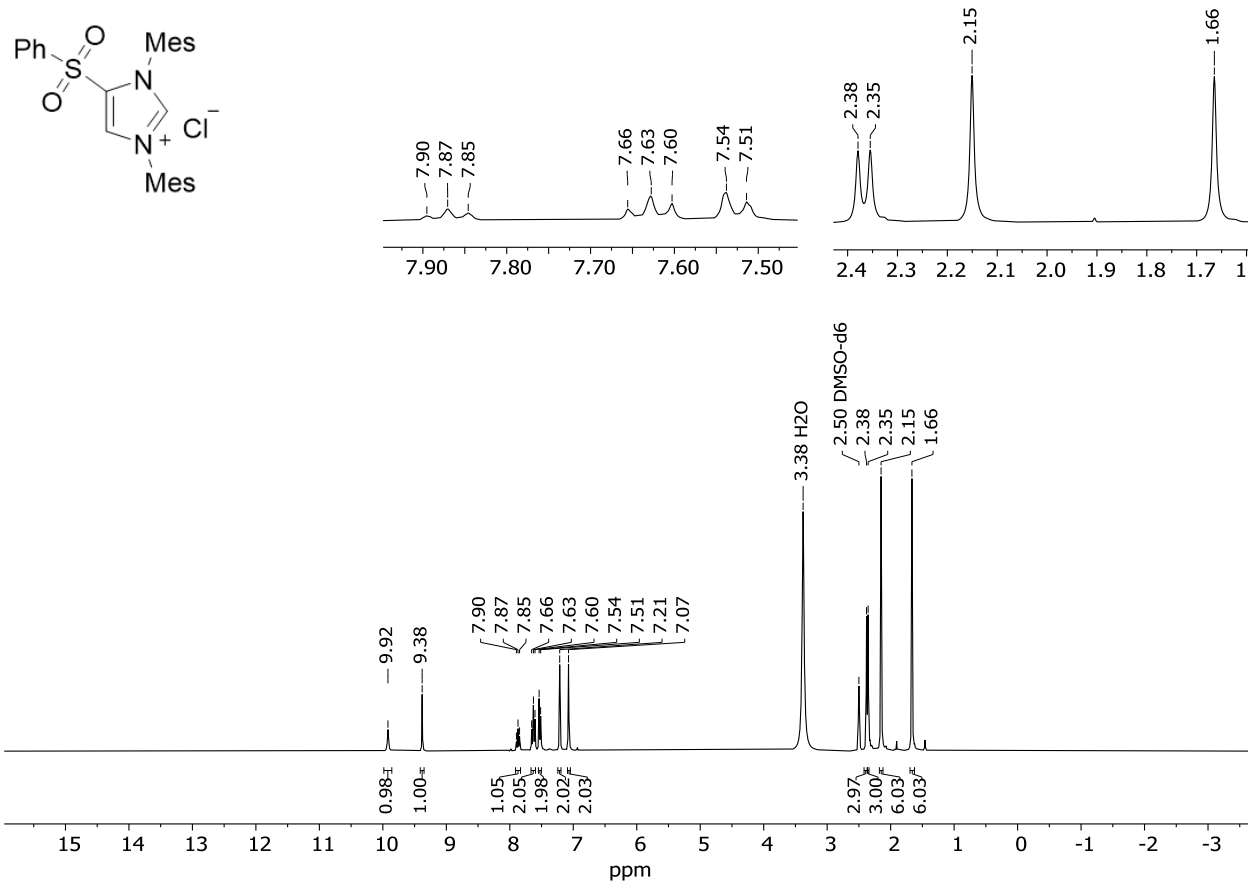


Figure S11. ^{1}H NMR spectrum of **2g** (DMSO-d_6, 300 MHz)

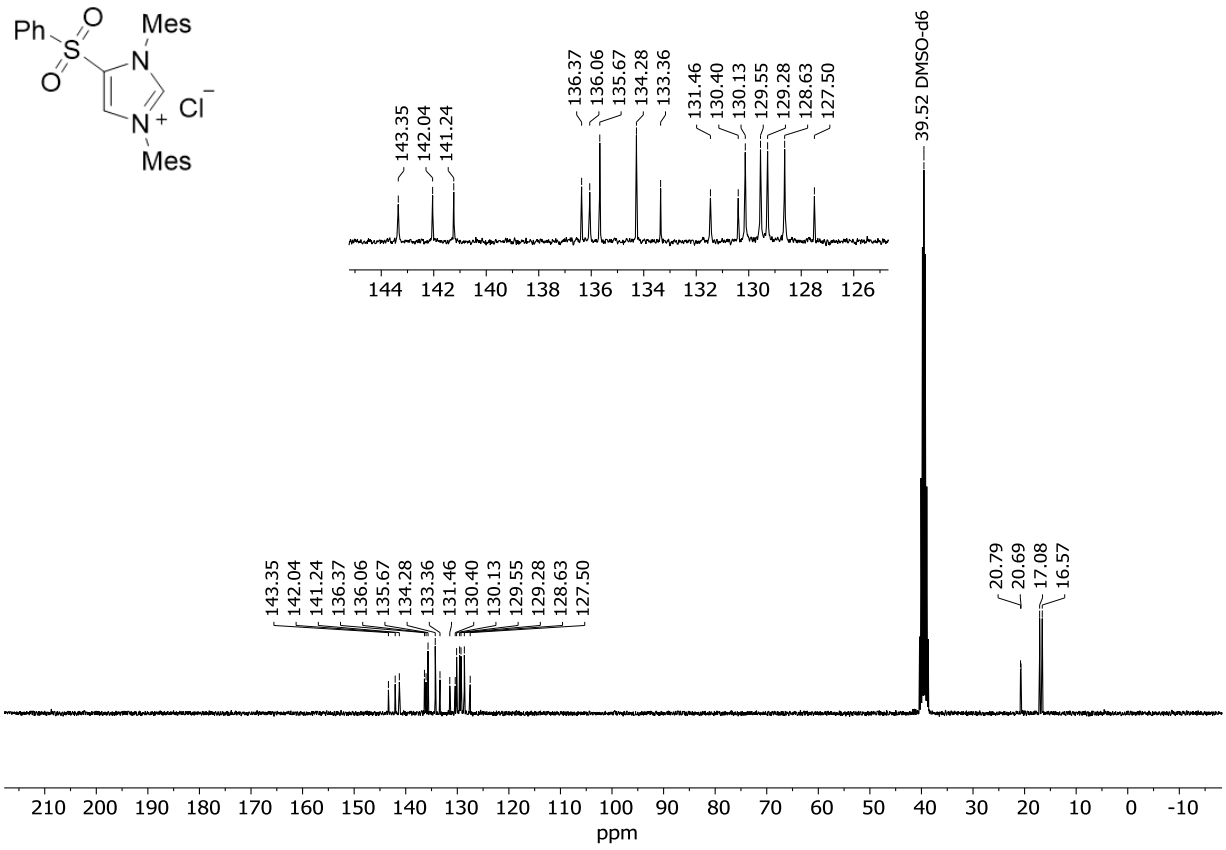


Figure S12. ^{13}C NMR spectrum of **2g** (DMSO-d_6, 75 MHz)

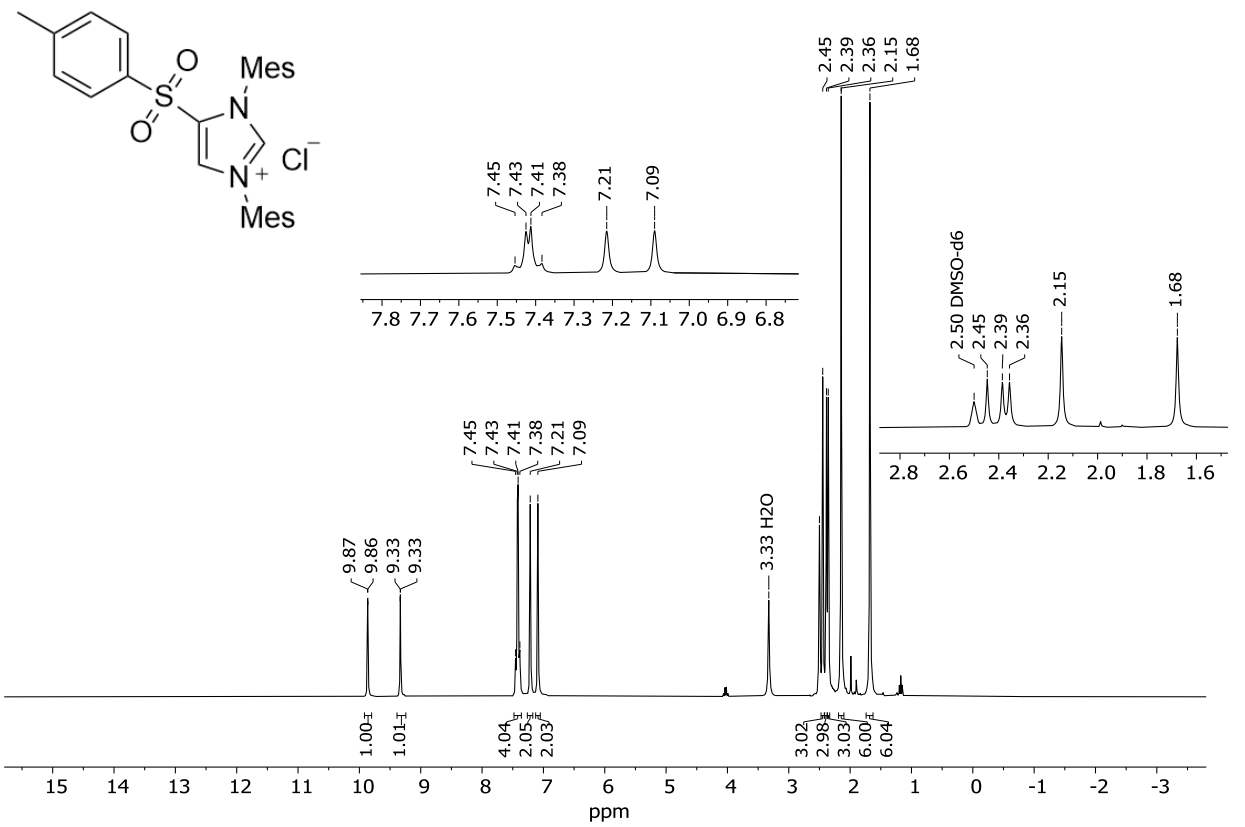


Figure S13. ^{1}H NMR spectrum of **2h** (DMSO-d_6, 300 MHz)

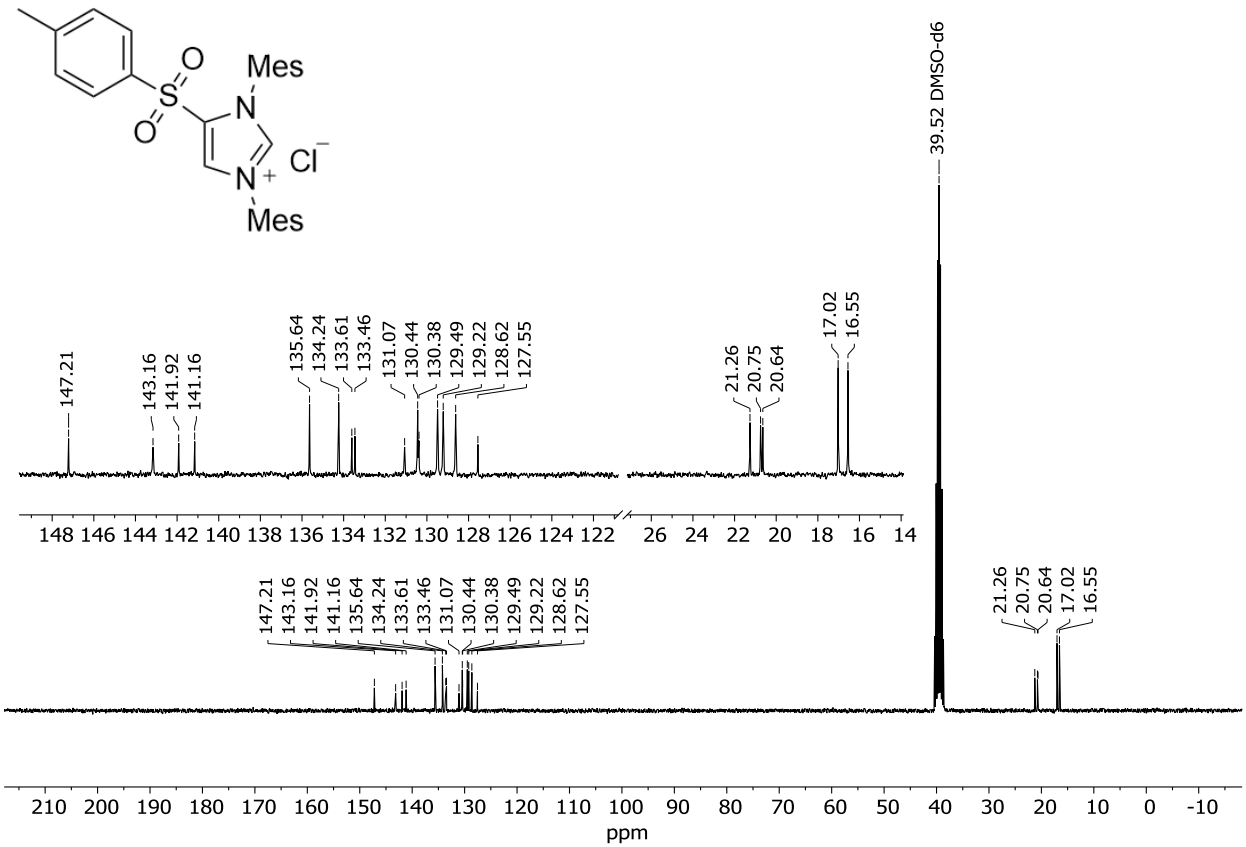


Figure S14. ^{13}C NMR spectrum of **2h** (DMSO-d_6, 75 MHz)

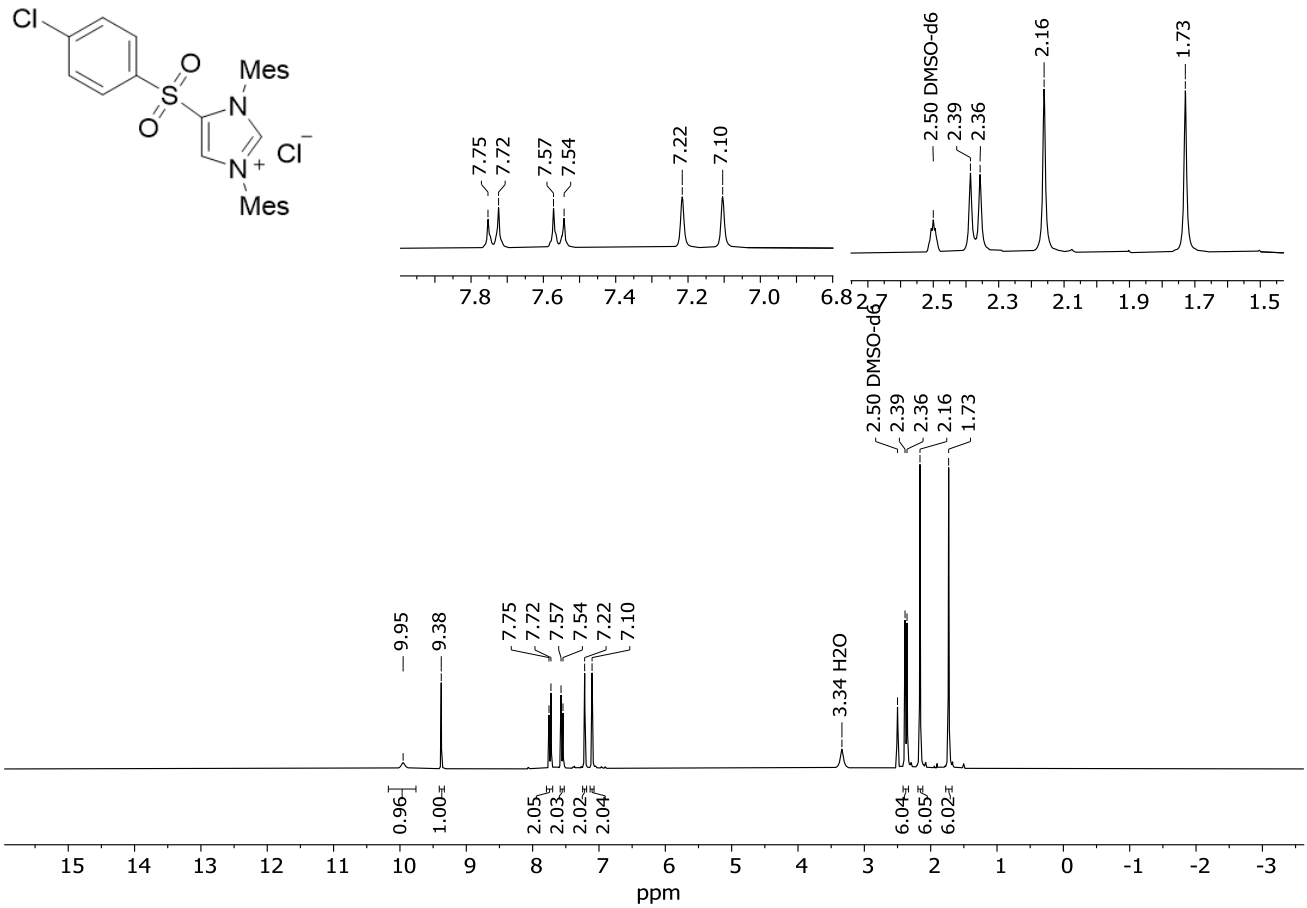


Figure S15. ^{1}H NMR spectrum of **2i** (DMSO-d_6, 300 MHz)

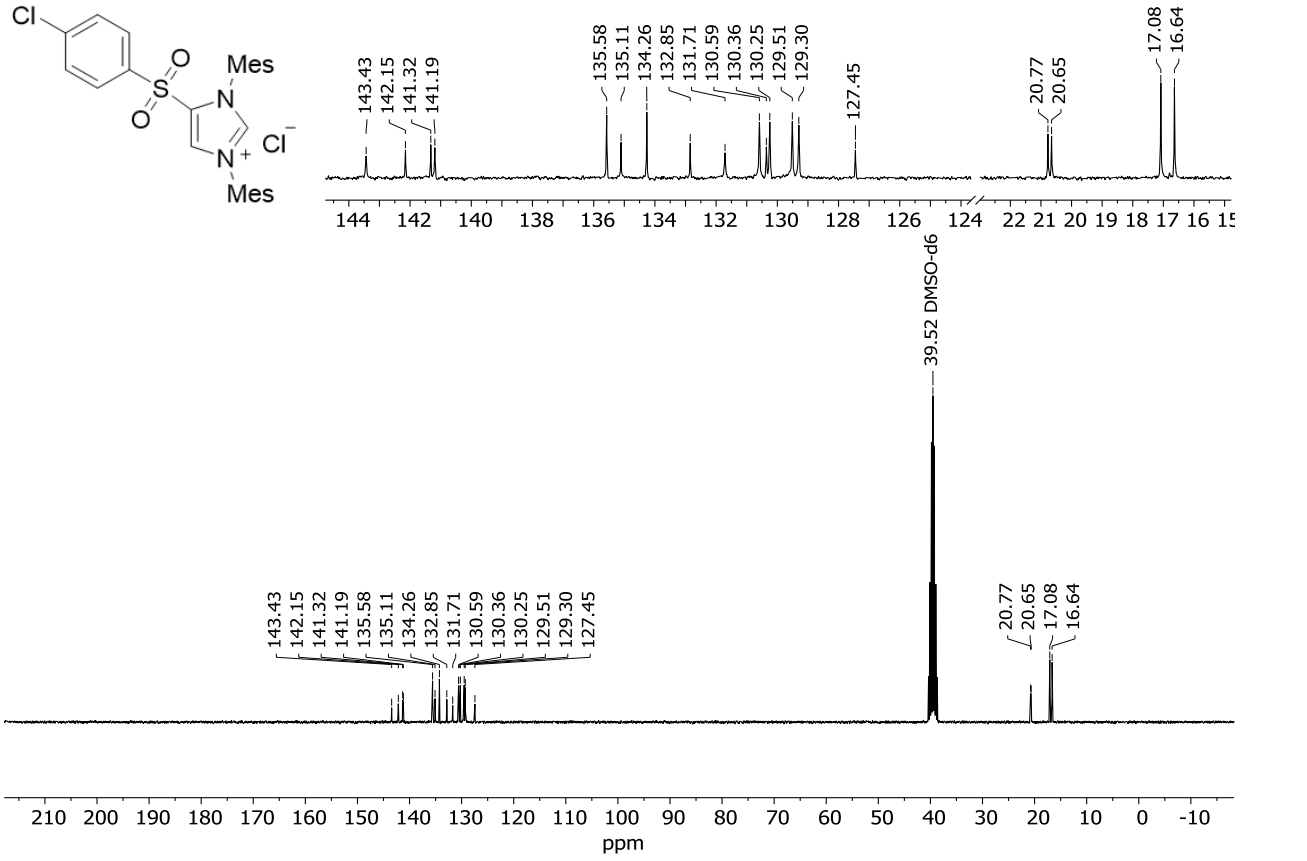


Figure S16. ^{13}C NMR spectrum of **2i** (DMSO-d_6, 75 MHz)

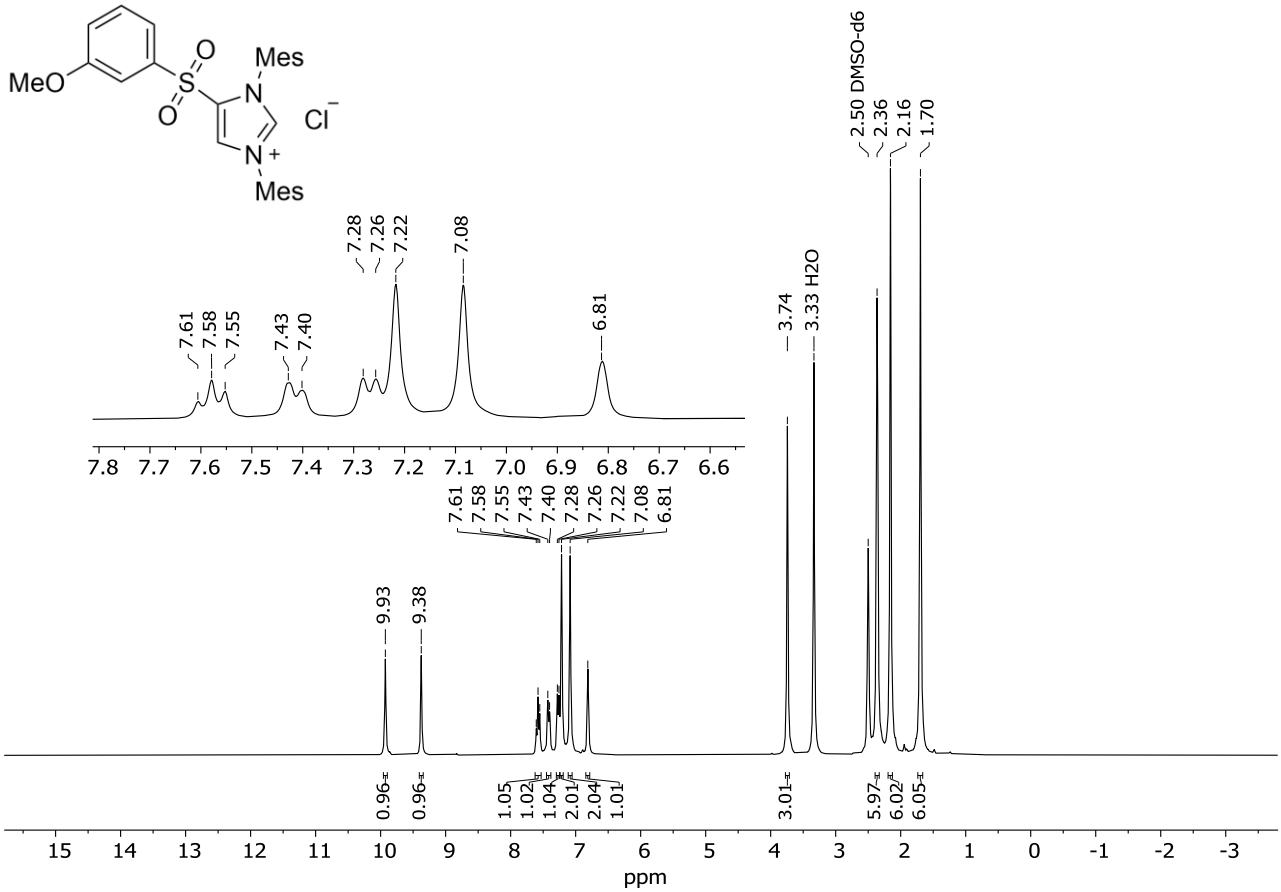


Figure S17. ^{1}H NMR spectrum of **2j** (DMSO-d_6, 300 MHz)

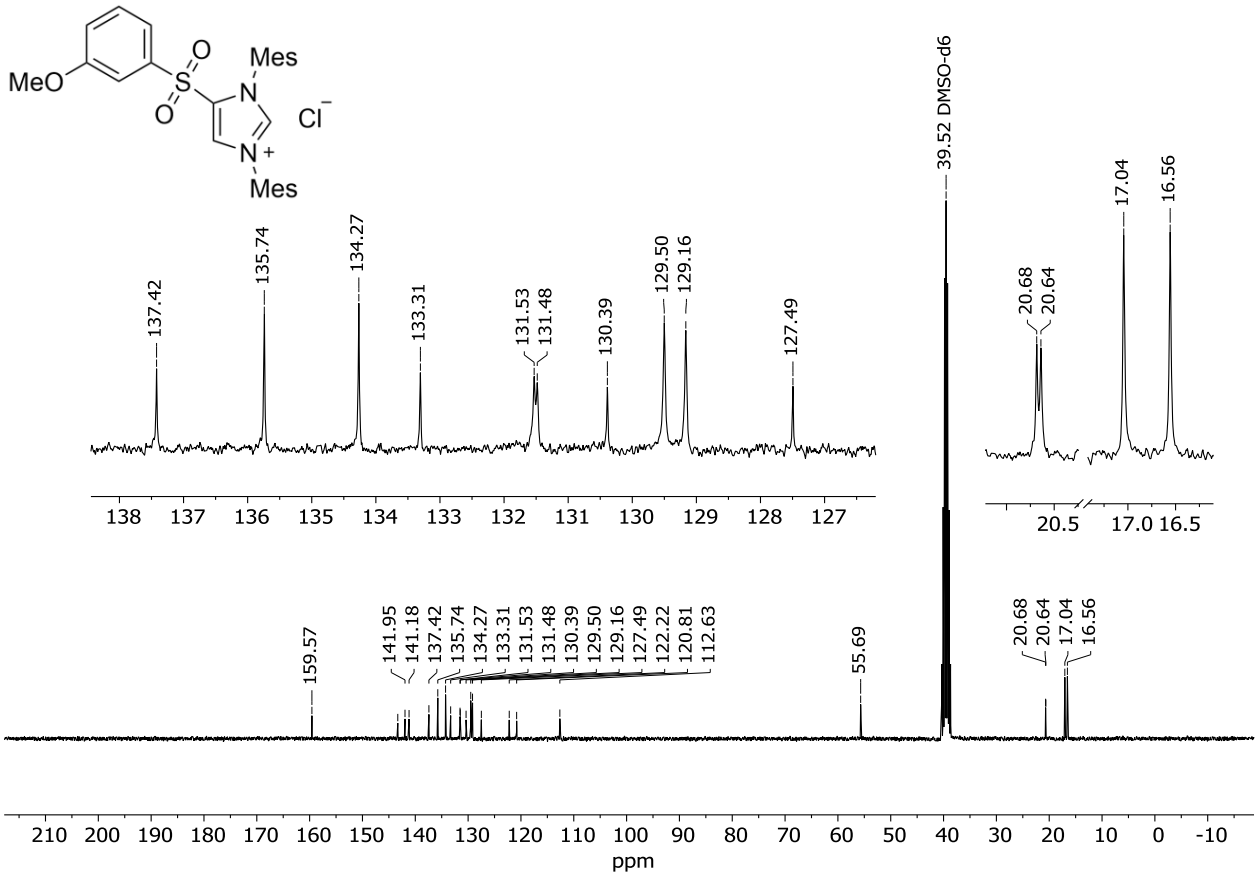


Figure S18. ^{13}C NMR spectrum of **2j** (DMSO-d_6, 75 MHz)

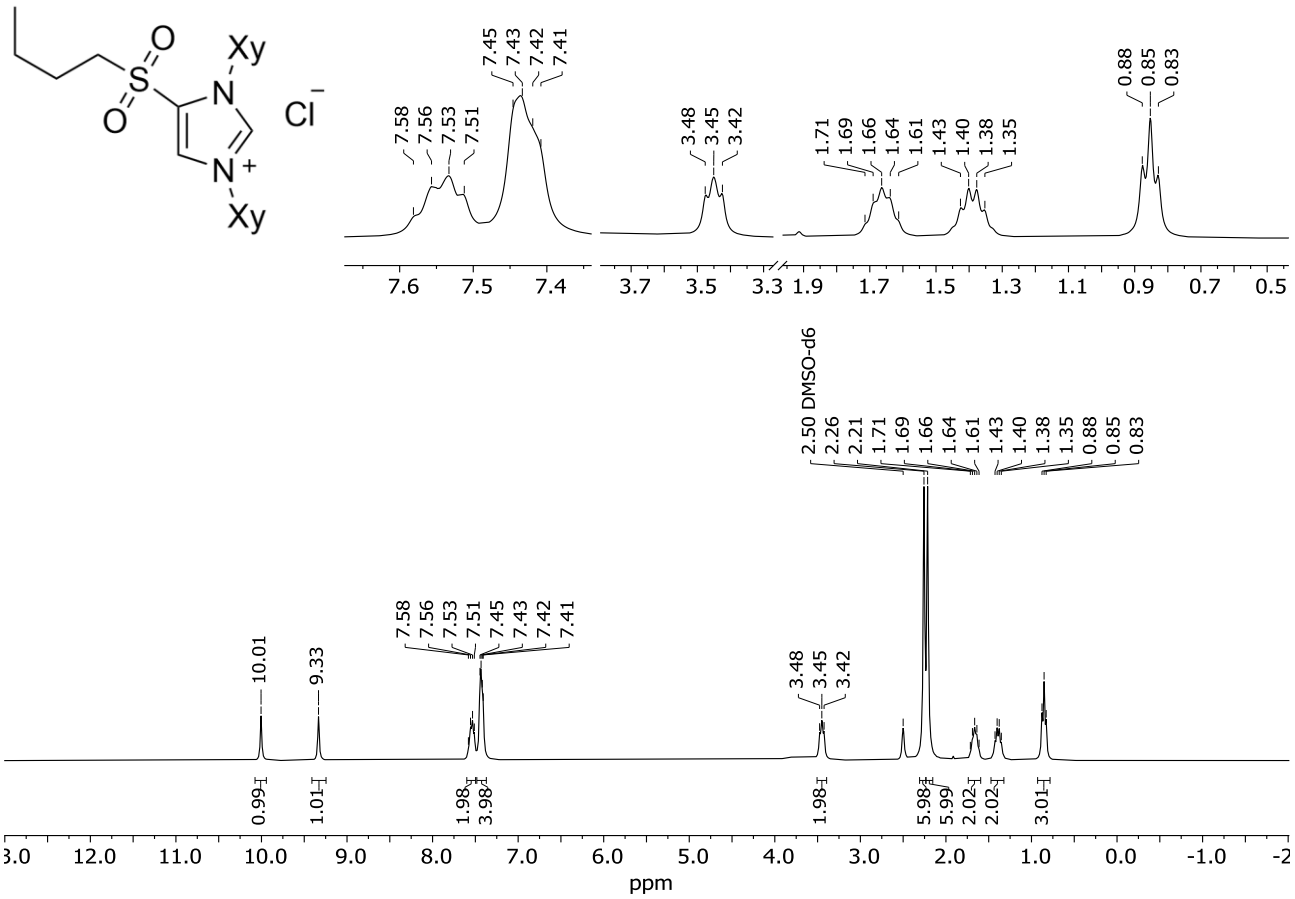


Figure S19. ^{1}H NMR spectrum of **2k** (DMSO-d_6, 300 MHz)

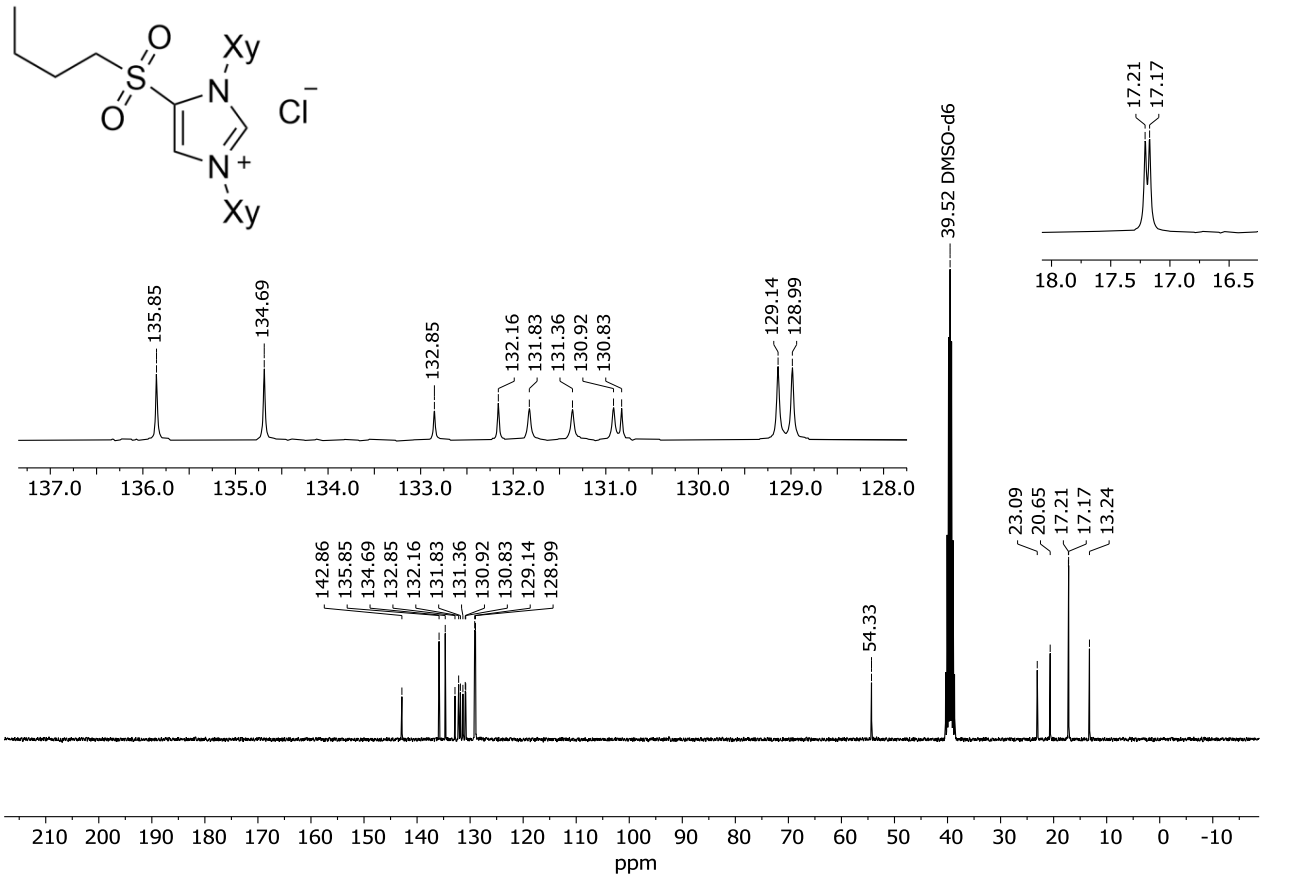


Figure S20. ^{13}C NMR spectrum of **2k** (DMSO-d_6, 75 MHz)

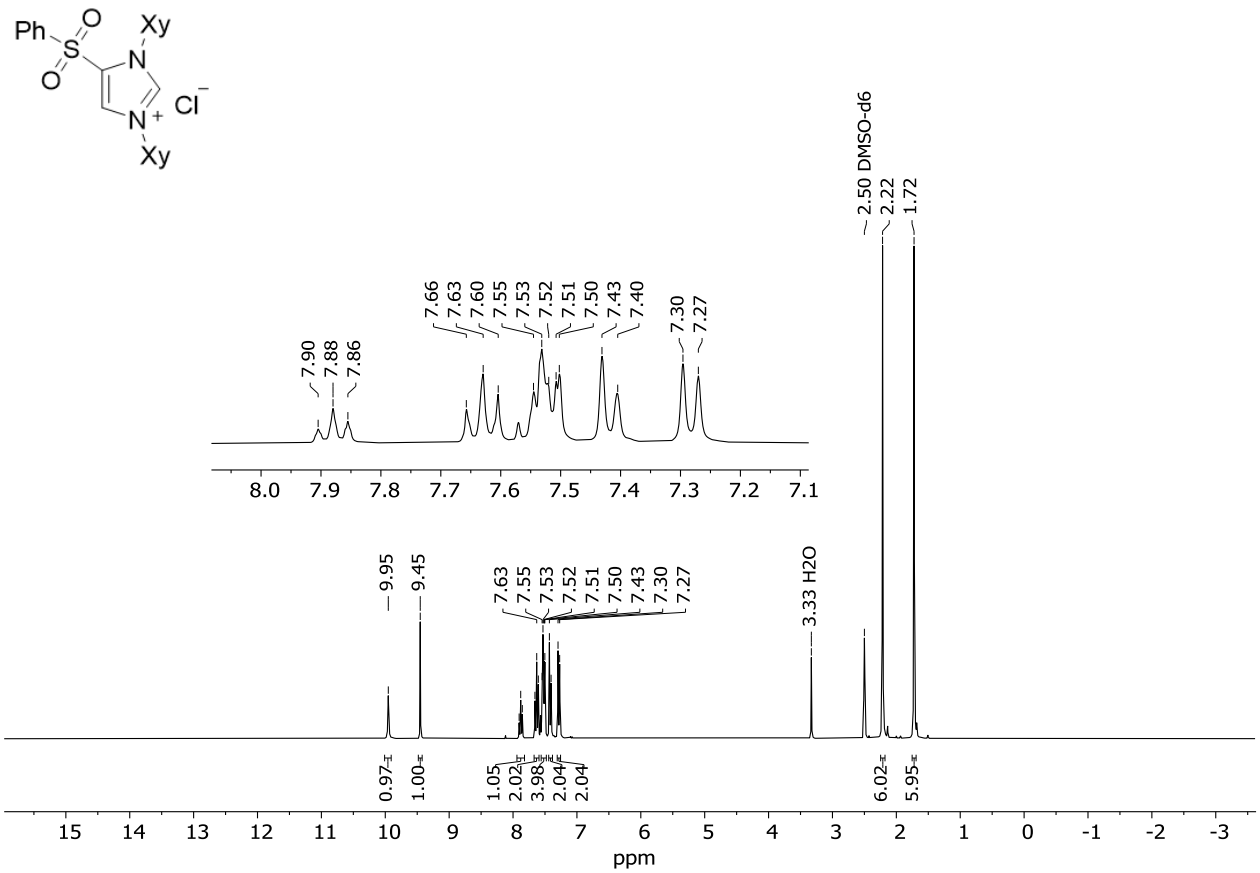


Figure S21. ^{1}H NMR spectrum of **2l** (DMSO-d_6, 300 MHz)

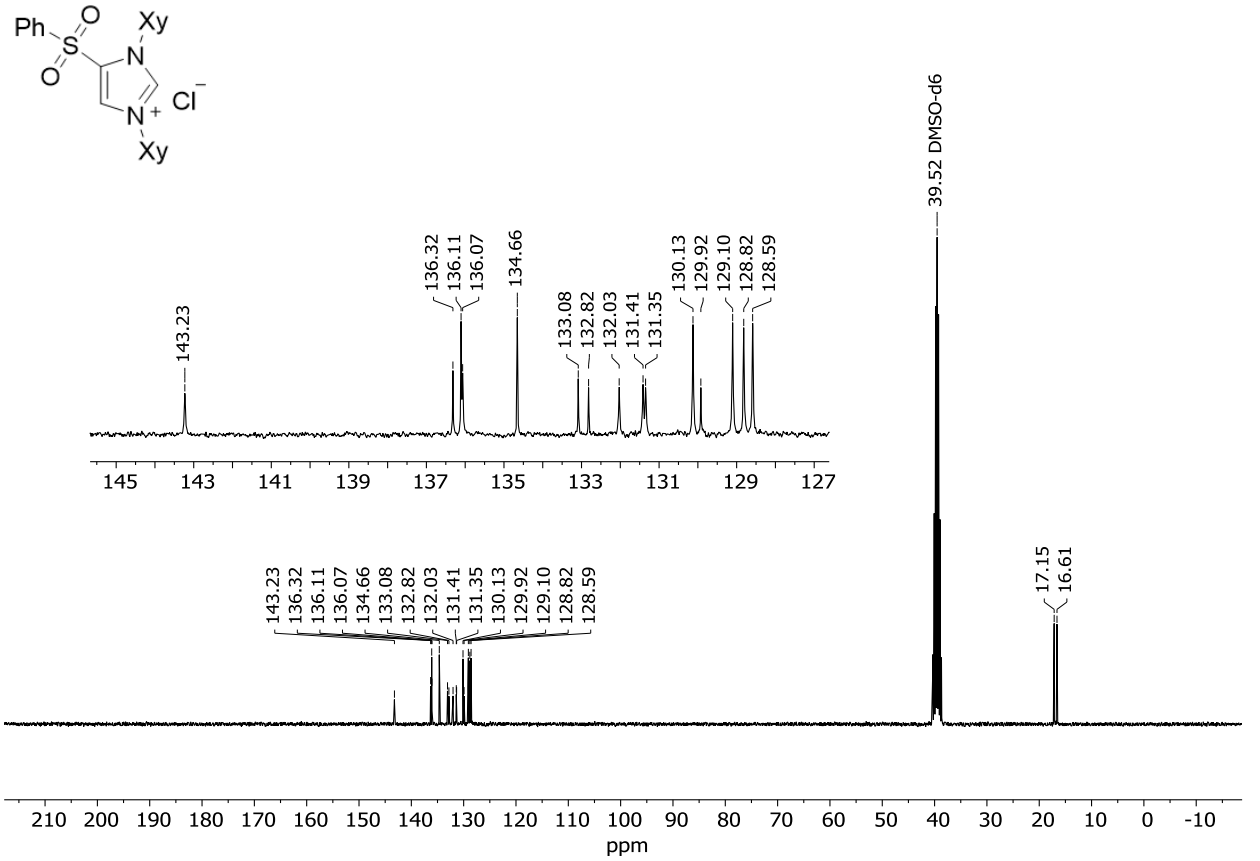


Figure S22. ^{13}C NMR spectrum of **2l** (DMSO-d_6, 75 MHz)

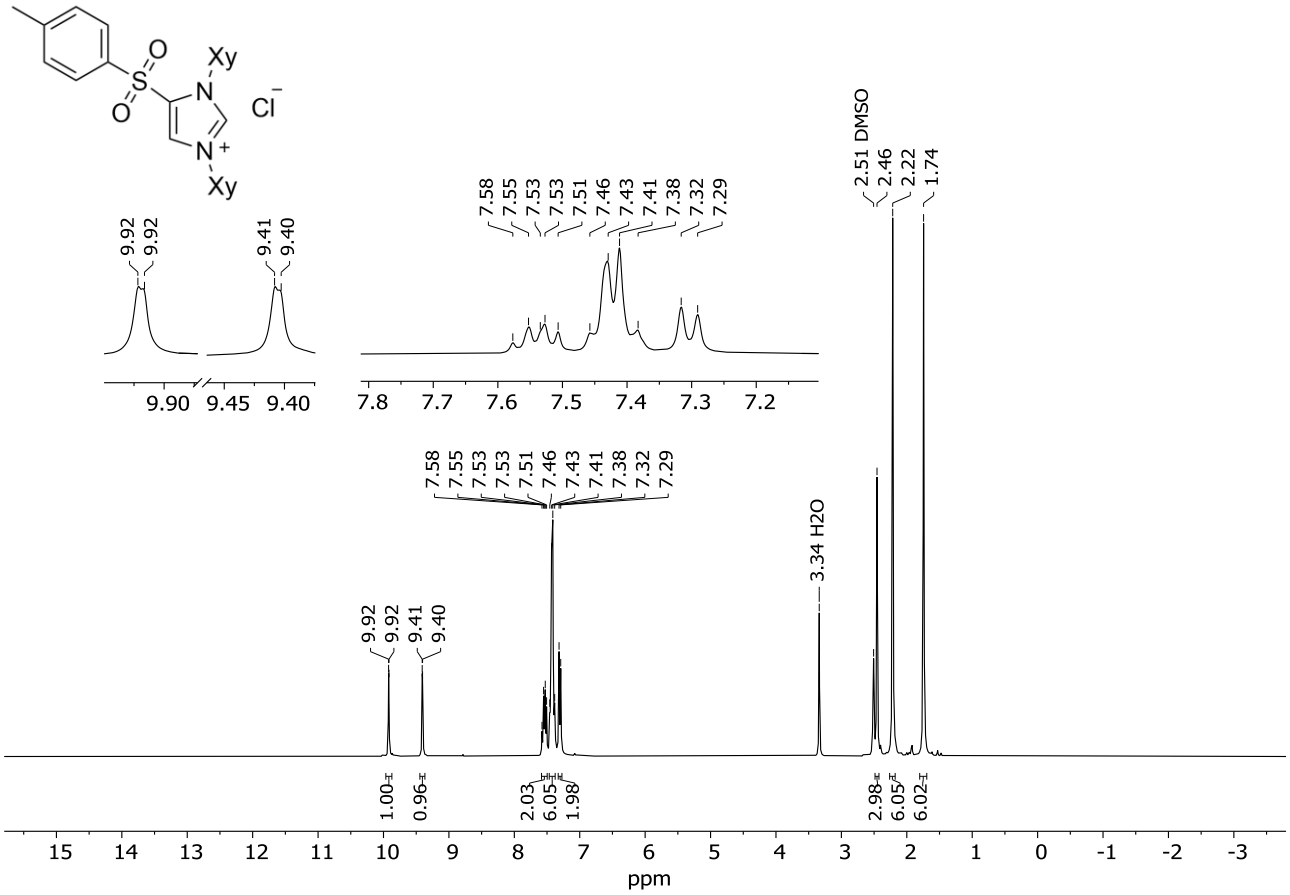


Figure S23. ^{1}H NMR spectrum of **2m** (DMSO-d_6, 300 MHz)

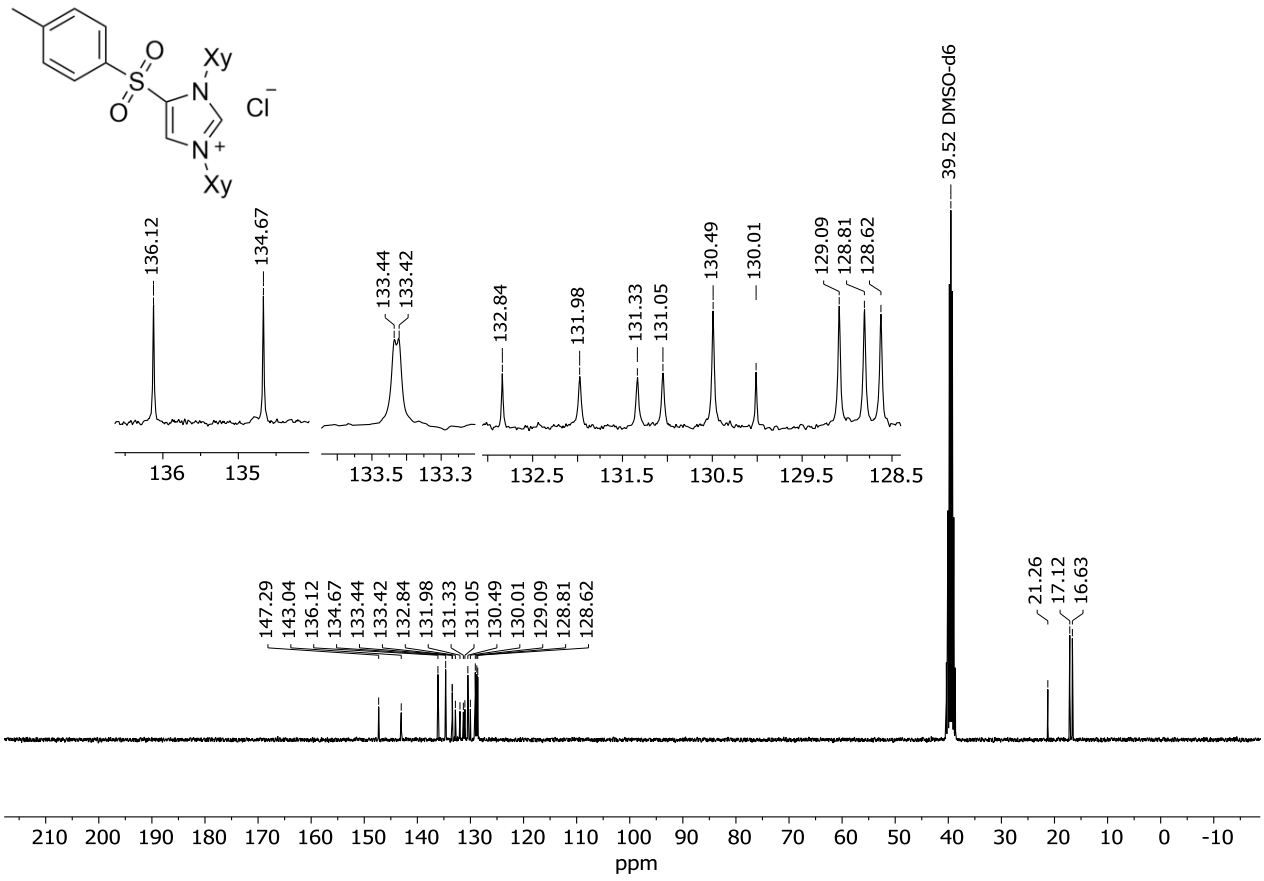


Figure S24. ^{13}C NMR spectrum of **2m** (DMSO-d_6, 75 MHz)

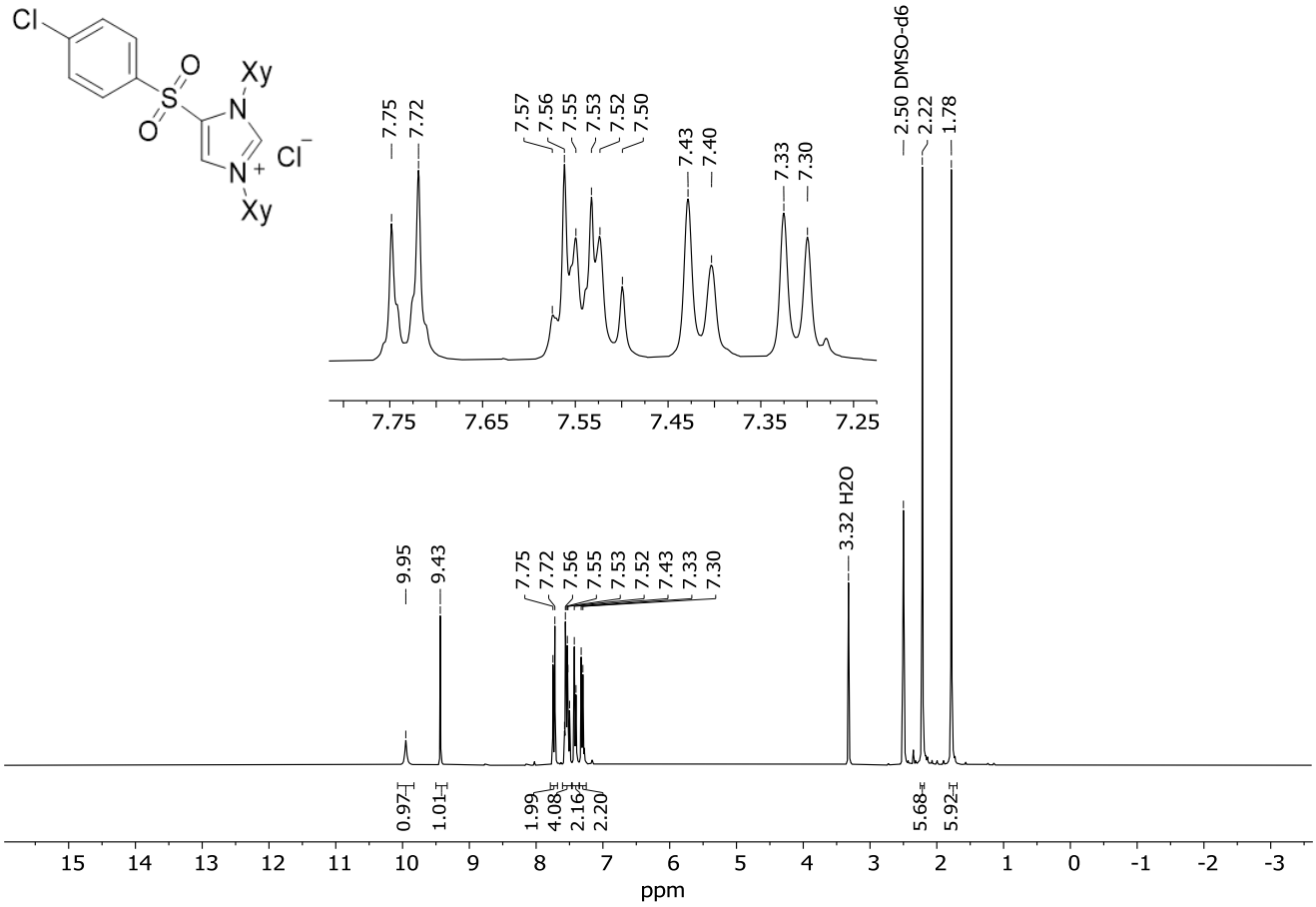


Figure S25. ^{1}H NMR spectrum of **2n** (DMSO-d_6, 300 MHz)

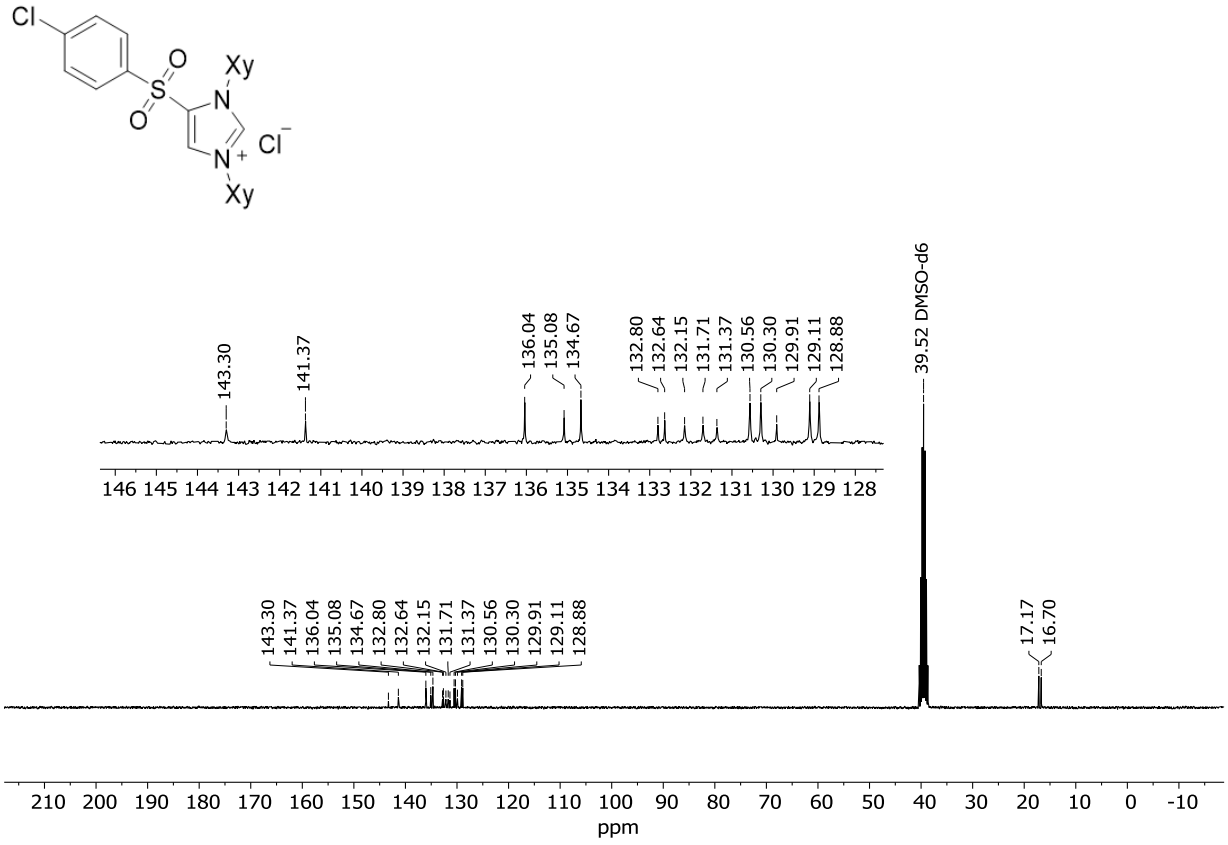


Figure S26. ^{13}C NMR spectrum of **2n** (DMSO-d_6, 75 MHz)

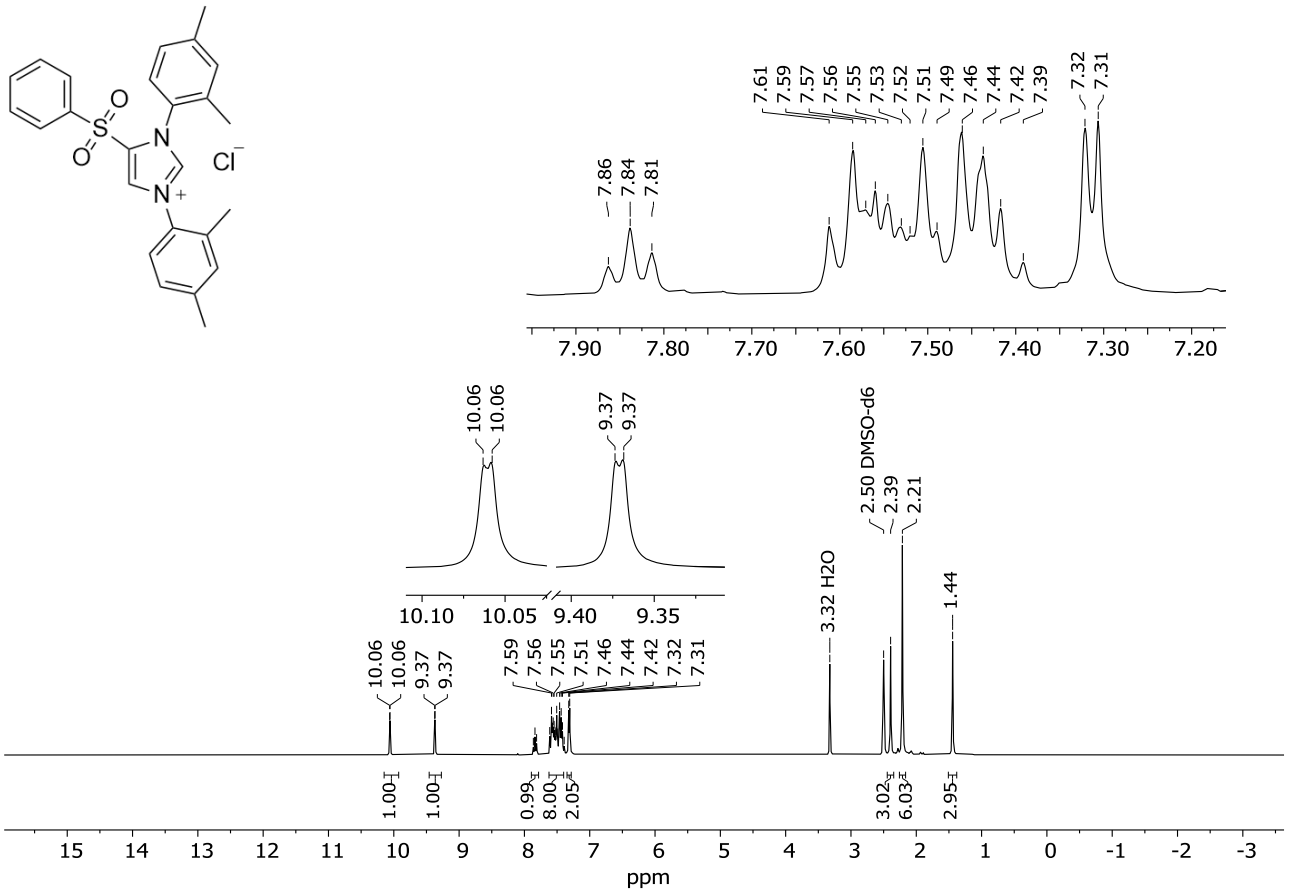


Figure S27. ^{1}H NMR spectrum of **2o** (DMSO-d_6, 300 MHz)

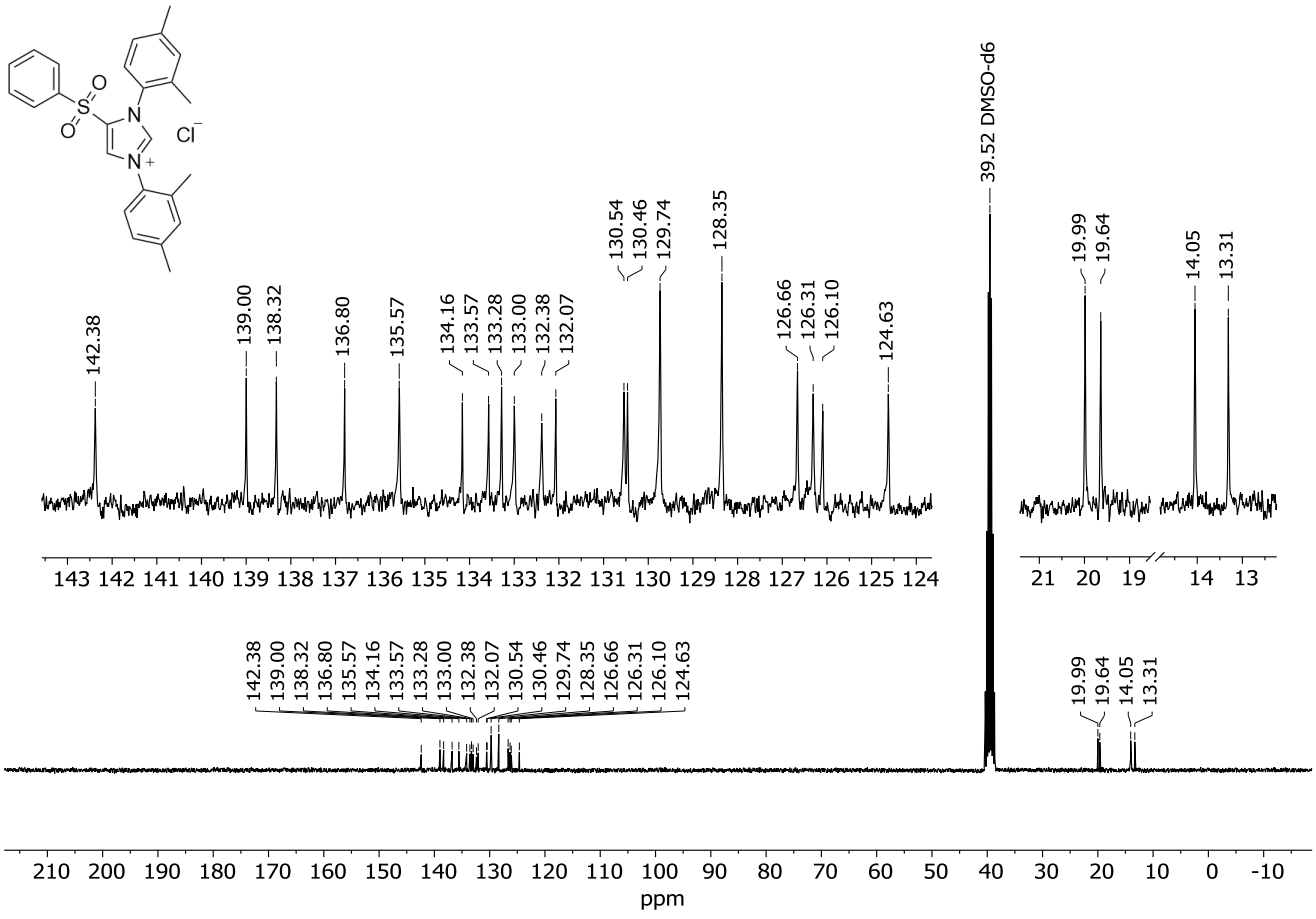


Figure S28. ^{13}C NMR spectrum of **2o** (DMSO-d_6, 75 MHz)

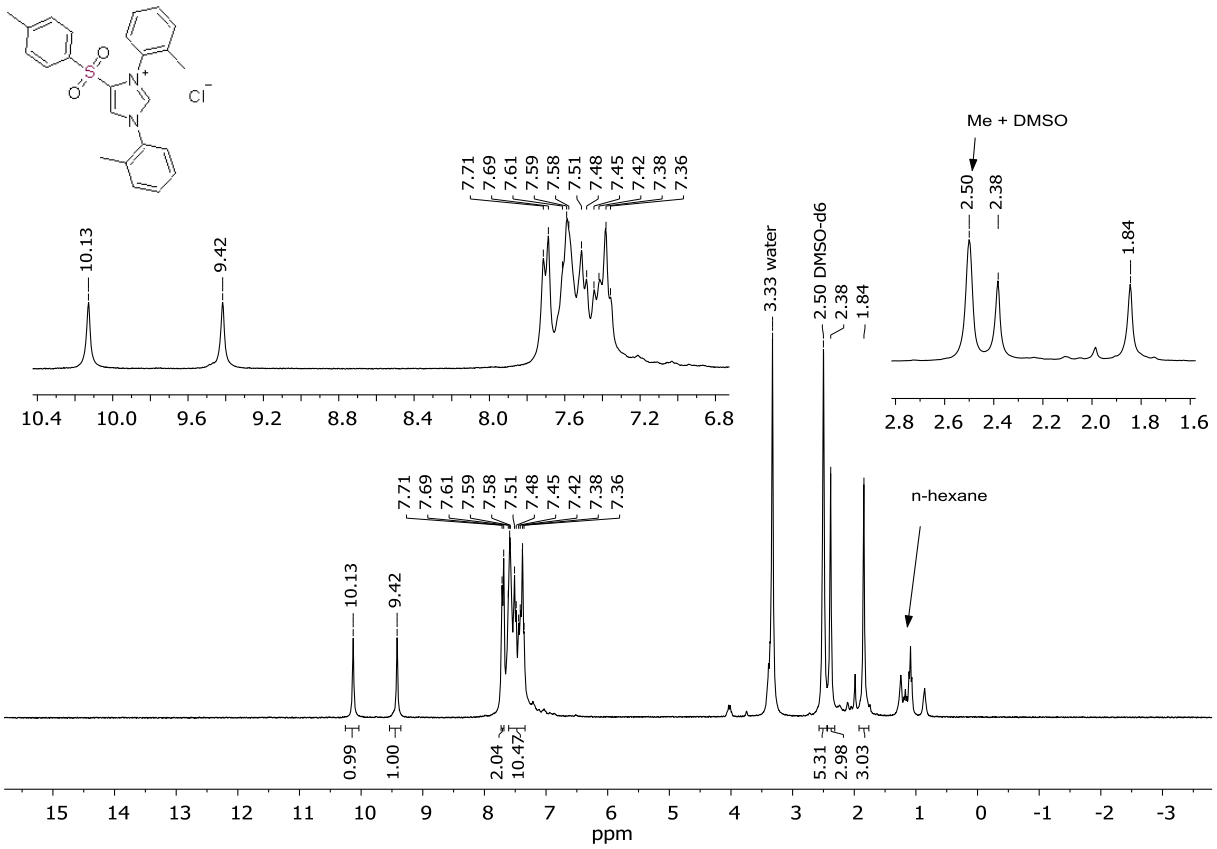


Figure S29. ^{1}H NMR spectrum of **2p** (DMSO-d_6, 300 MHz)

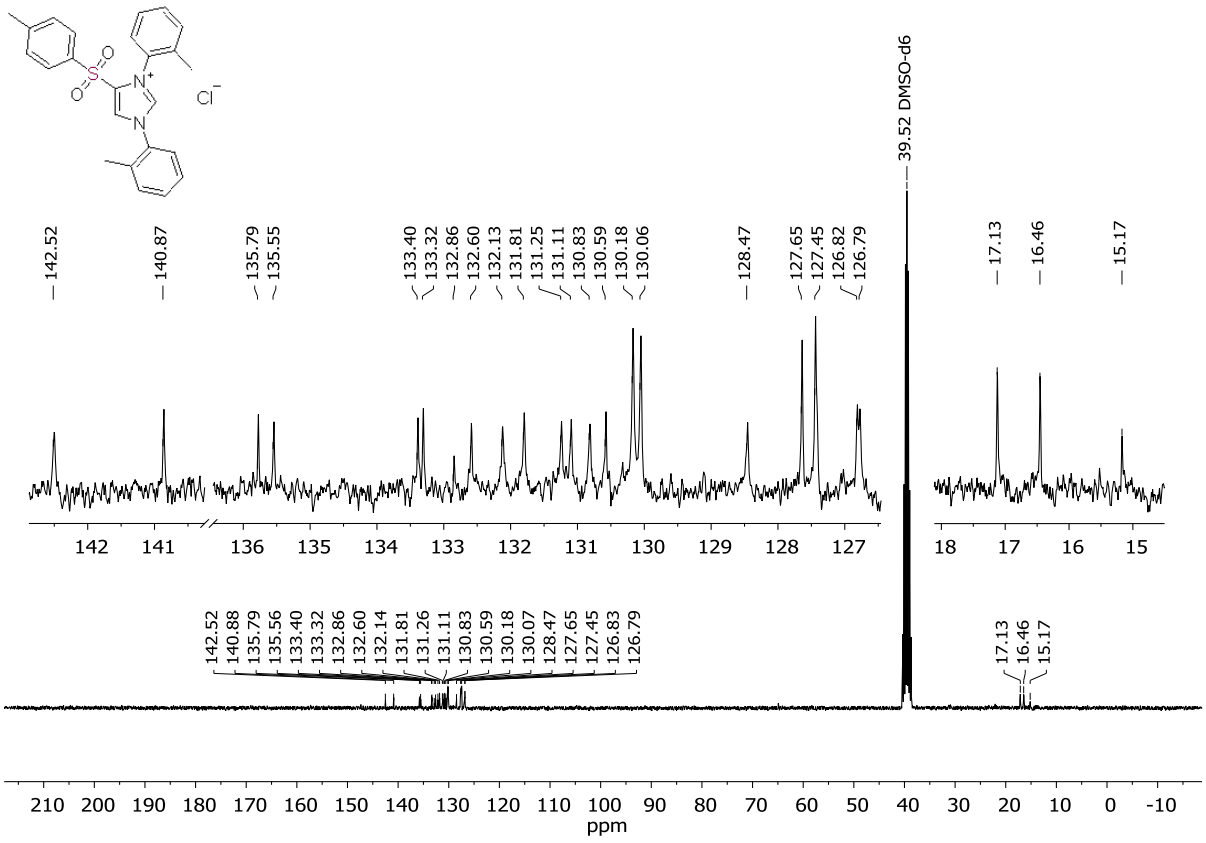


Figure S30. ^{13}C NMR spectrum of **2p** (DMSO-d_6, 75 MHz)

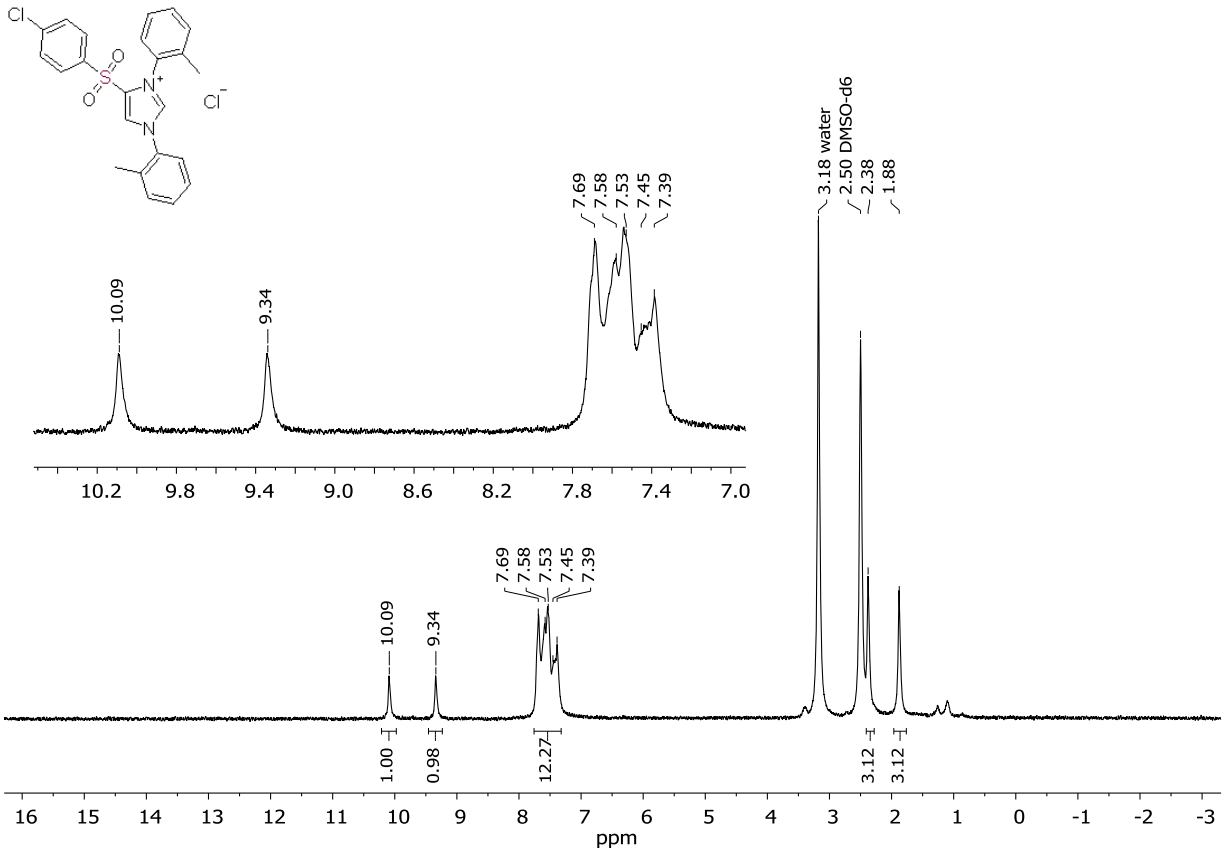


Figure S31. ^{1}H NMR spectrum of **2q** (DMSO-d_6, 300 MHz)

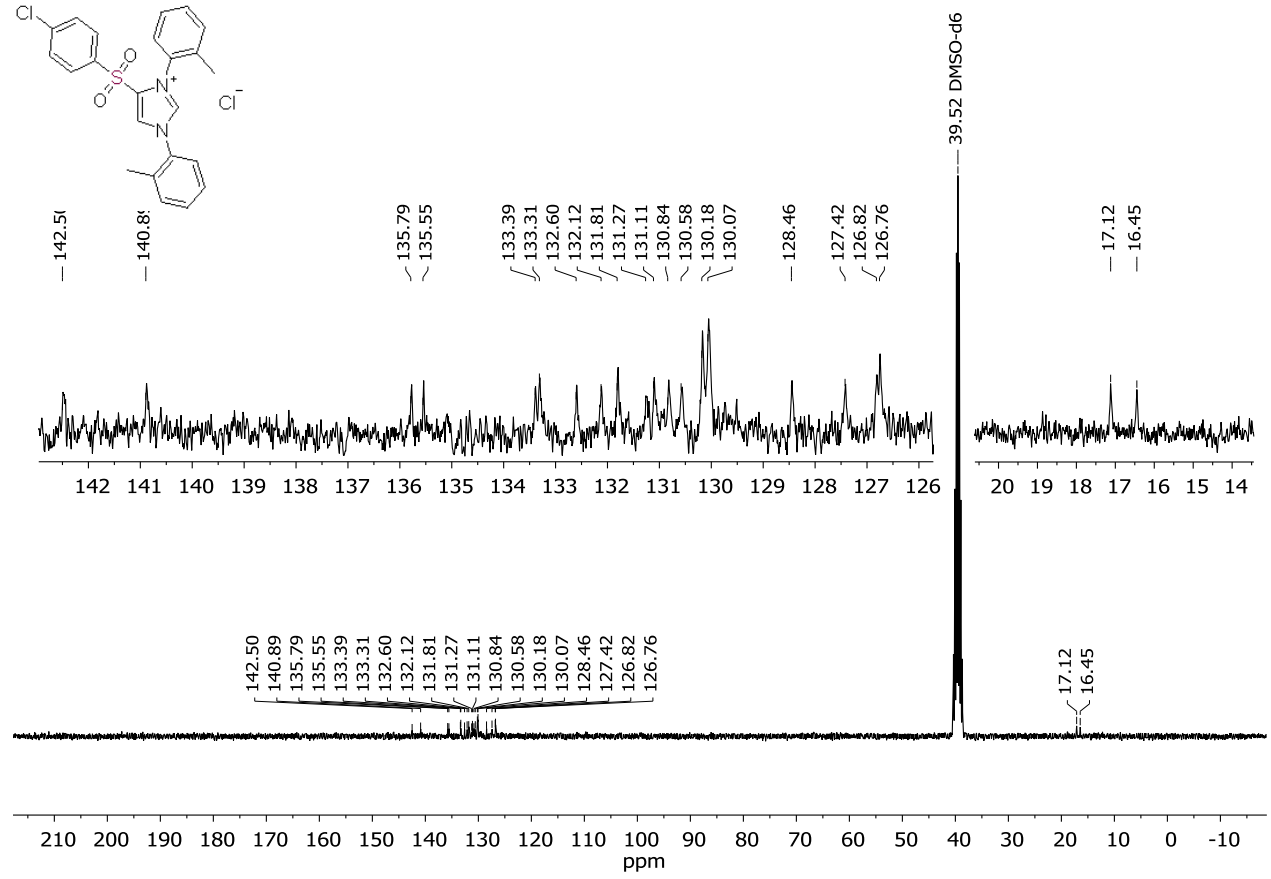


Figure S32. ^{13}C NMR spectrum of **2q** (DMSO-d_6, 75 MHz)

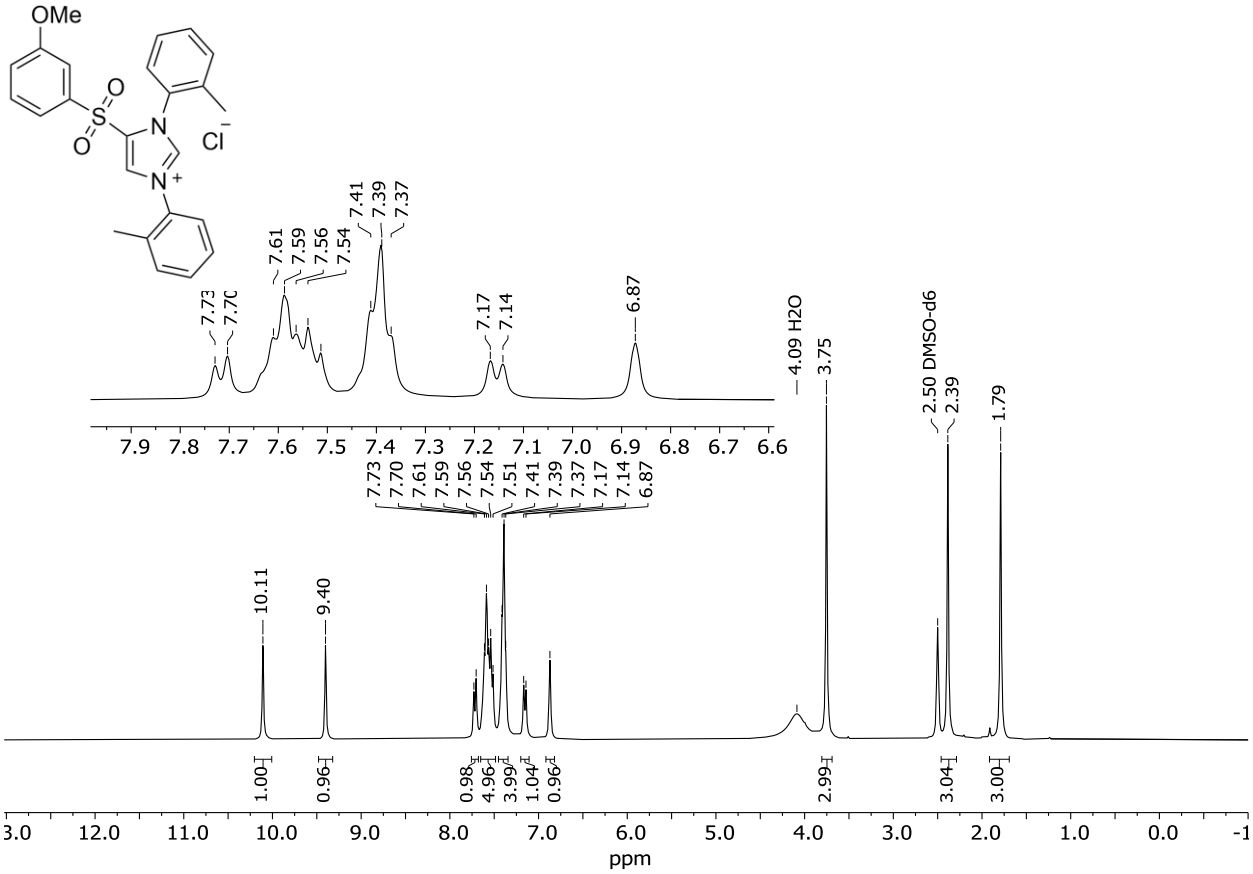


Figure S33. ^{1}H NMR spectrum of **2r** (DMSO-d_6, 300 MHz)

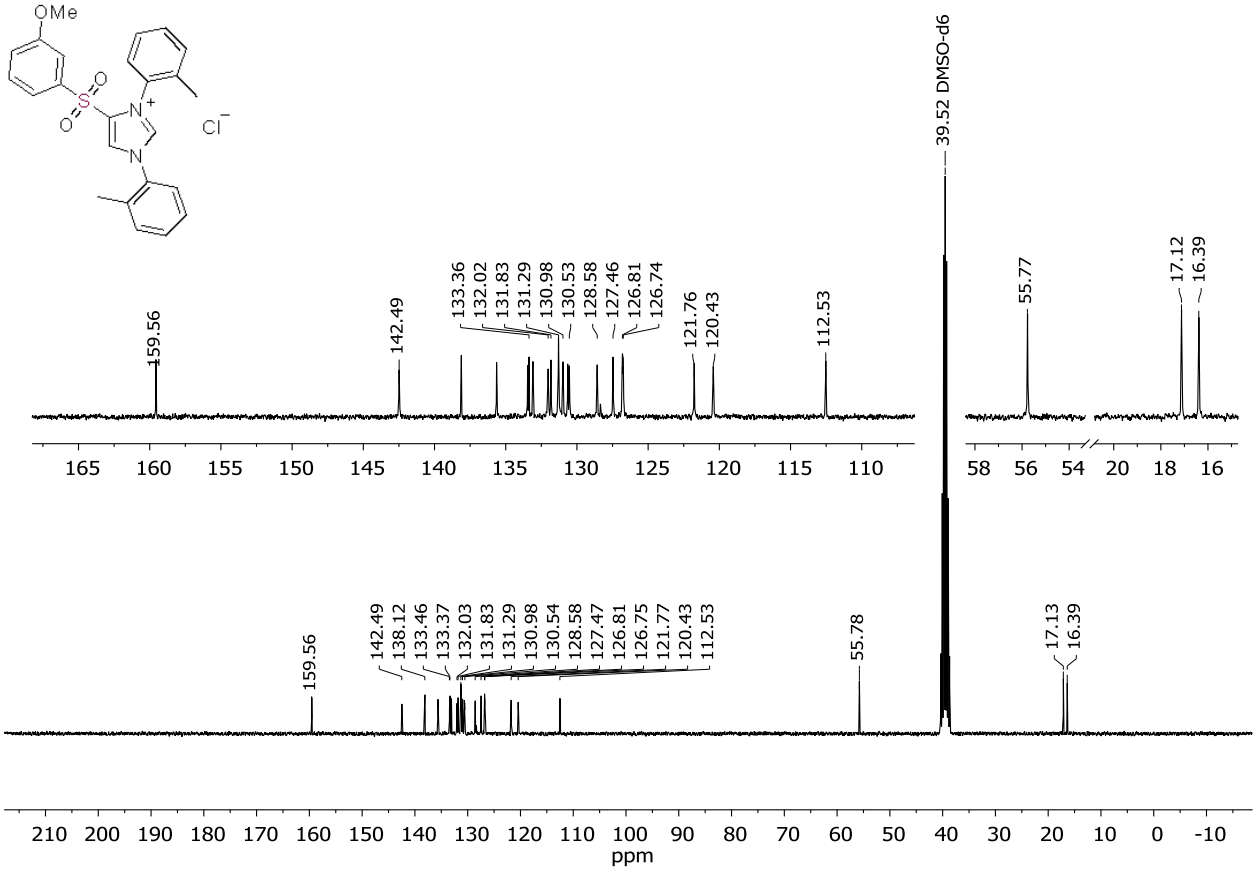


Figure S34. ^{13}C NMR spectrum of **2r** (DMSO-d_6, 75 MHz)

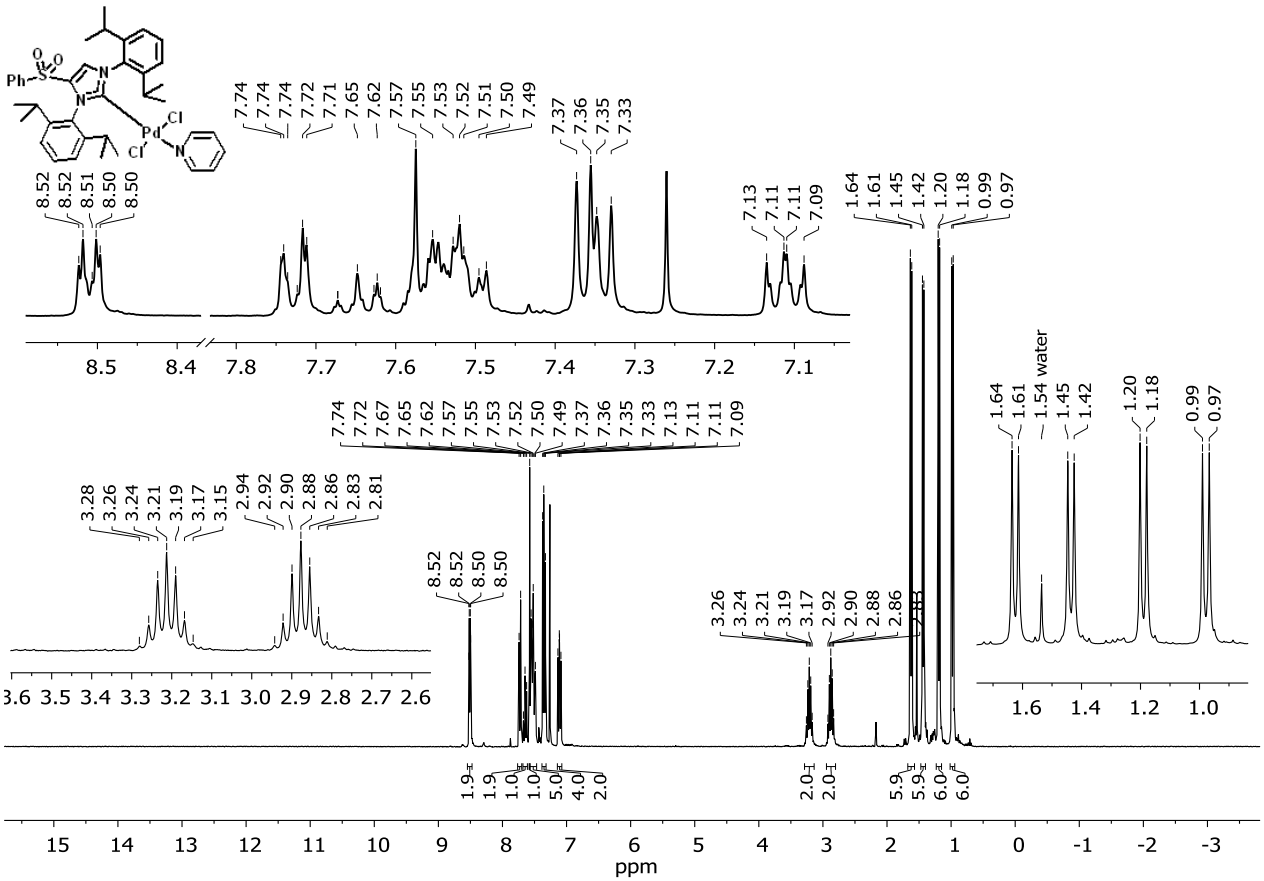


Figure S35. ^{1}H NMR spectrum of **3a** ($CDCl_3$, 300 MHz)

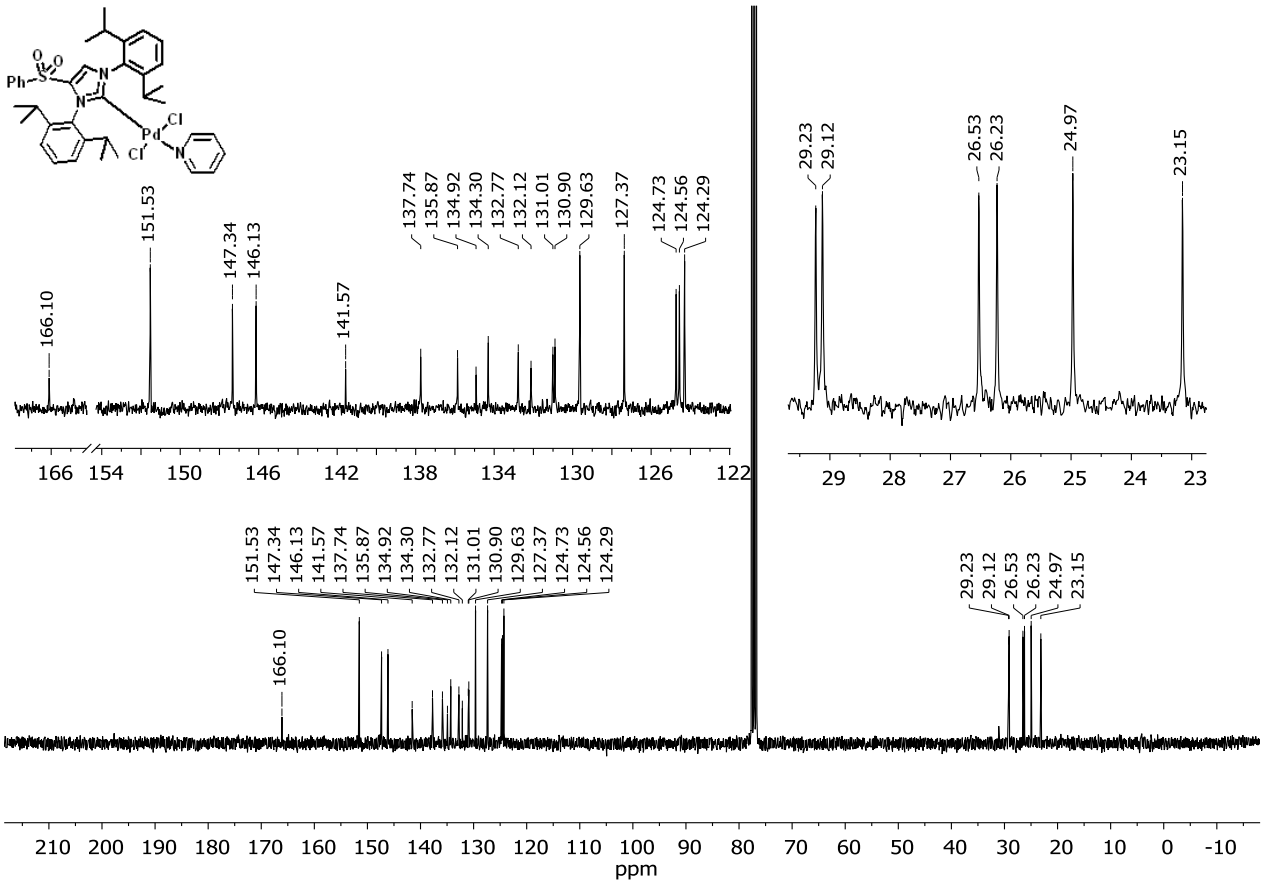


Figure S36. ^{13}C NMR spectrum of **3a** ($CDCl_3$, 75 MHz)

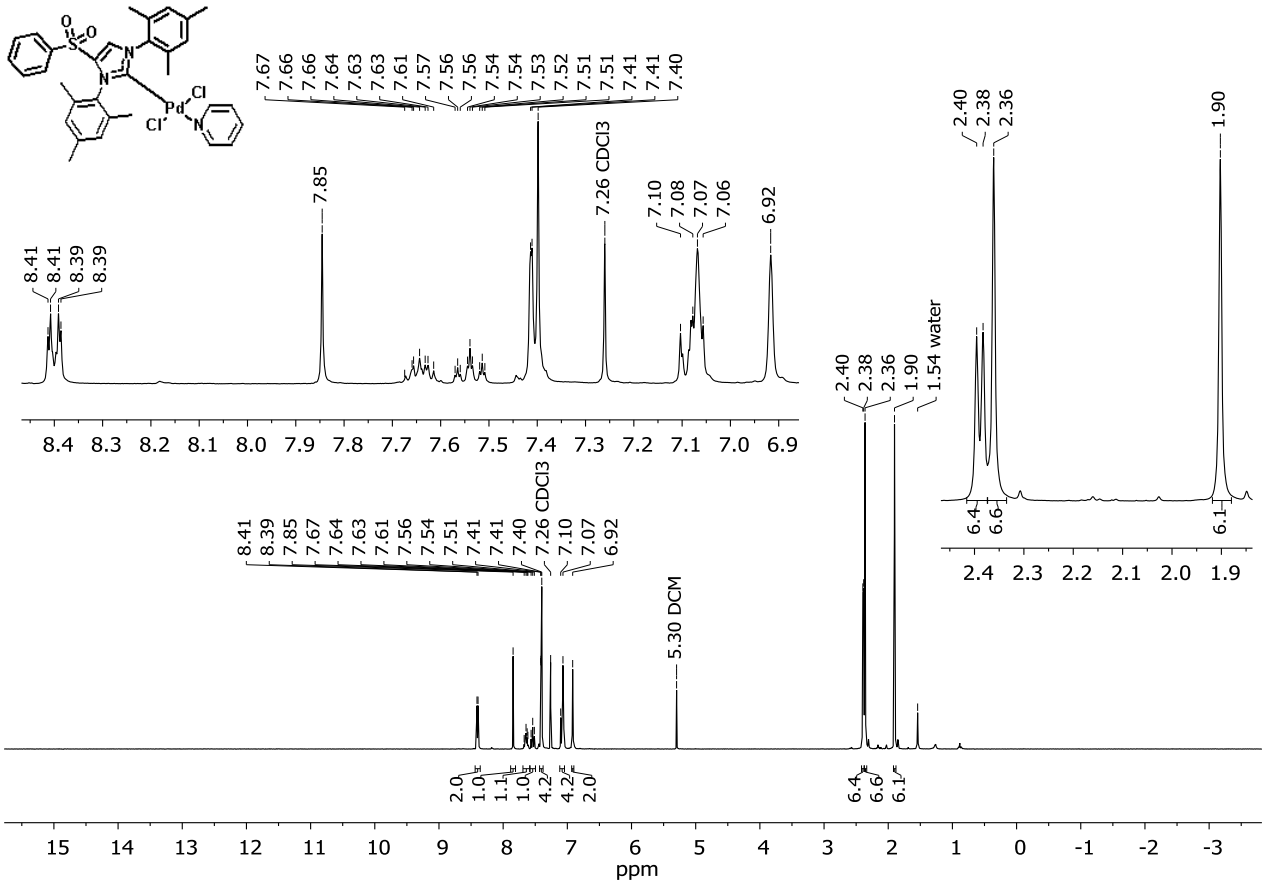


Figure S37. ^{1}H NMR spectrum of **3b** ($CDCl_3$, 300 MHz)

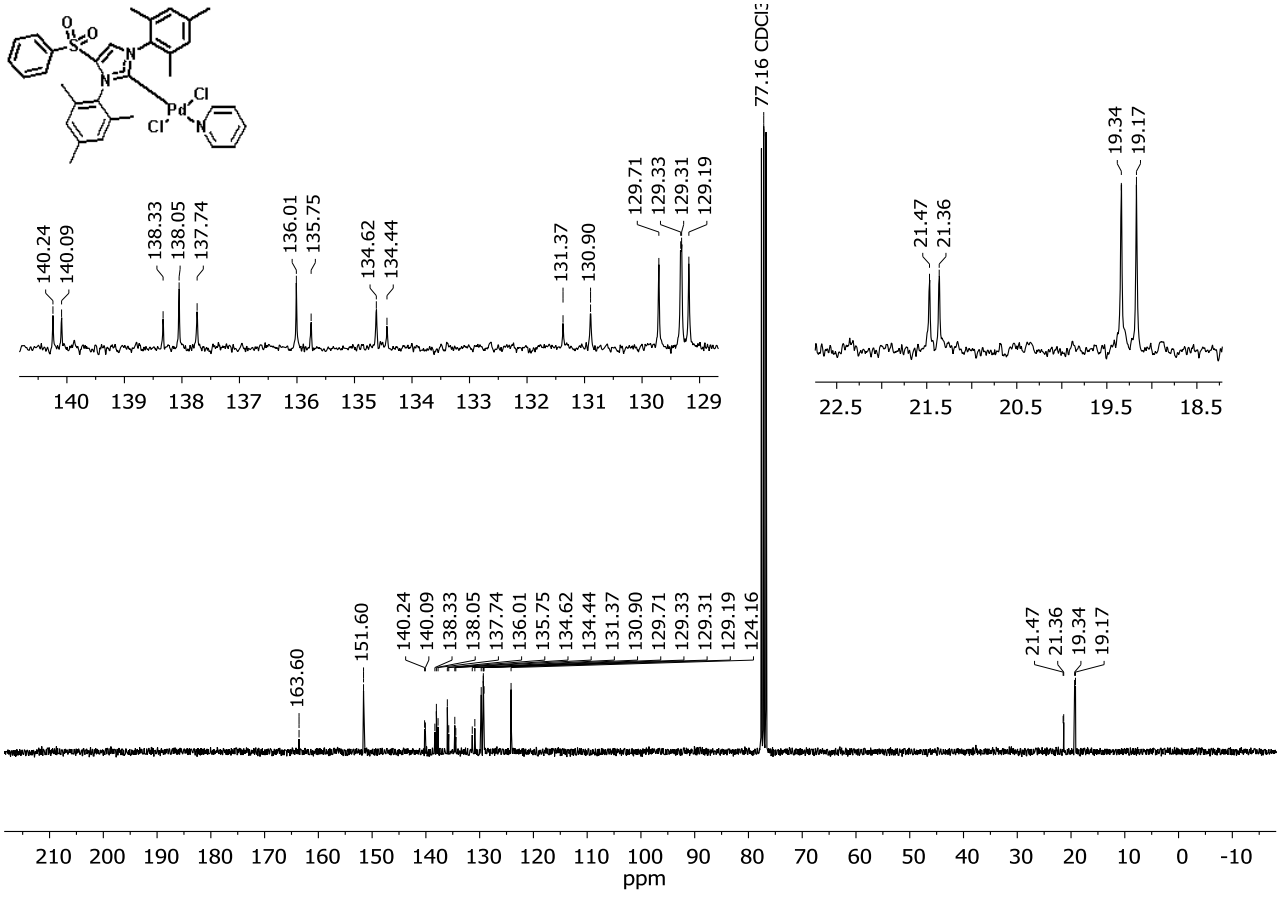


Figure S38. ^{13}C NMR spectrum of **3b** ($CDCl_3$, 75 MHz)

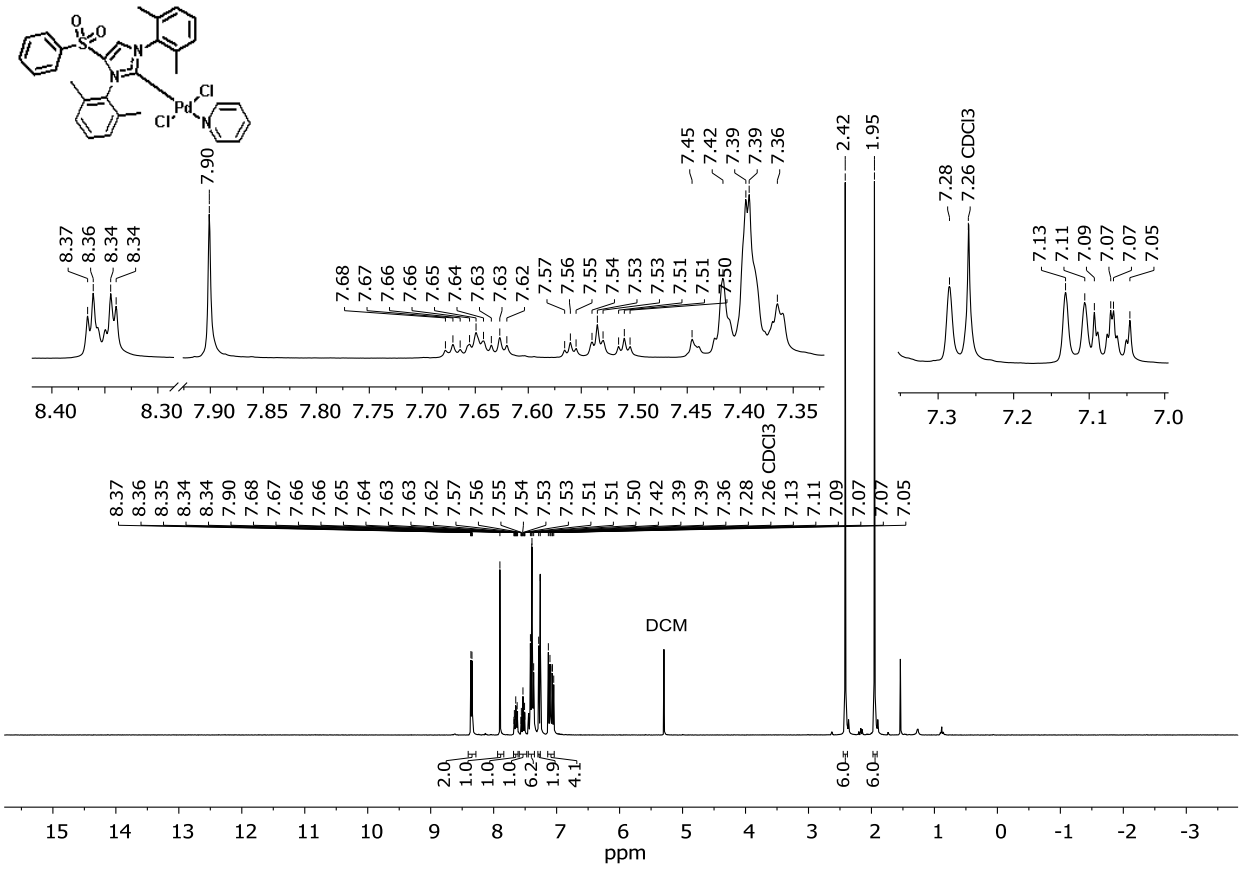


Figure S39. ^{1}H NMR spectrum of **3c** ($CDCl_3$, 300 MHz)

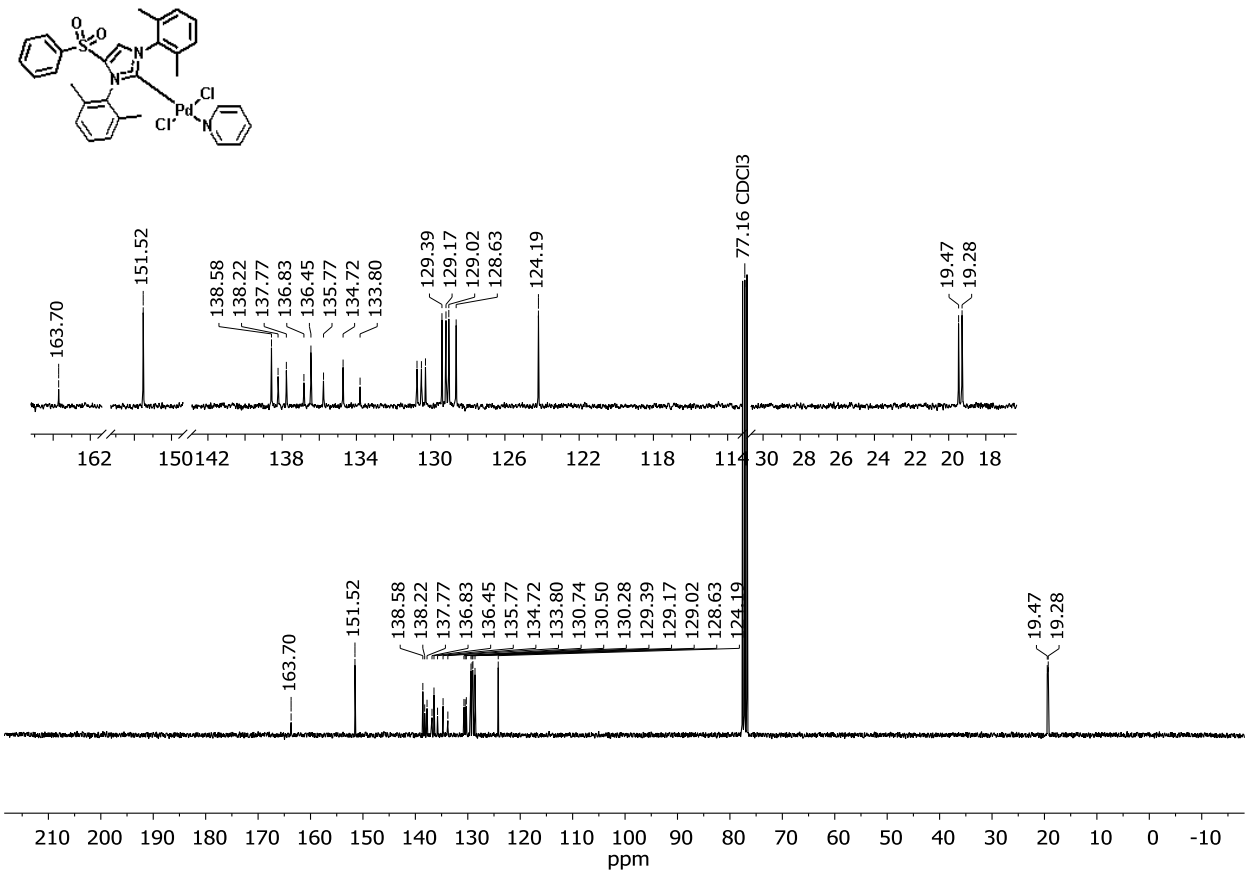


Figure S40. ^{13}C NMR spectrum of **3c** ($CDCl_3$, 75 MHz)

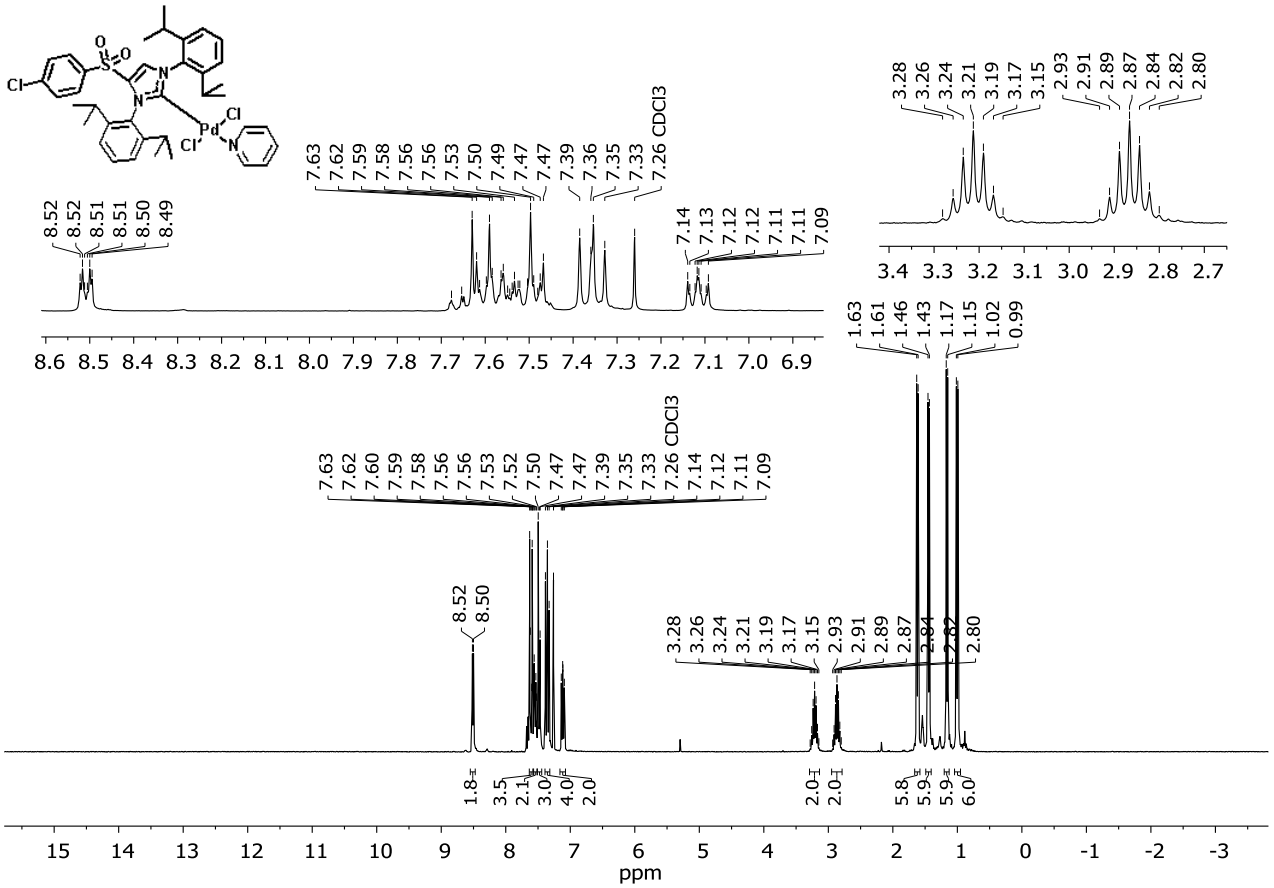


Figure S41. ^{1}H NMR spectrum of **3d** ($CDCl_3$, 300 MHz)

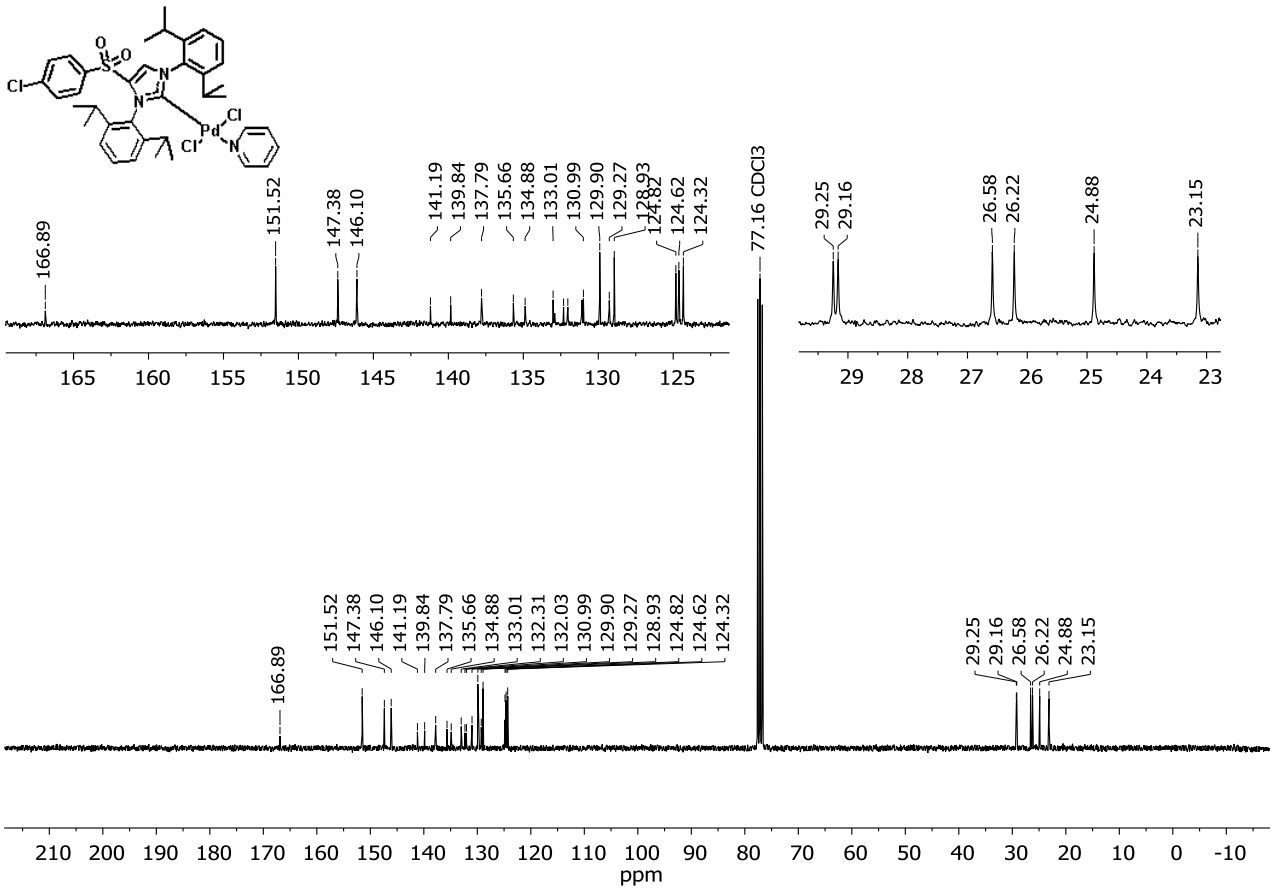


Figure S42. ^{13}C NMR spectrum of **3d** ($CDCl_3$, 75 MHz)

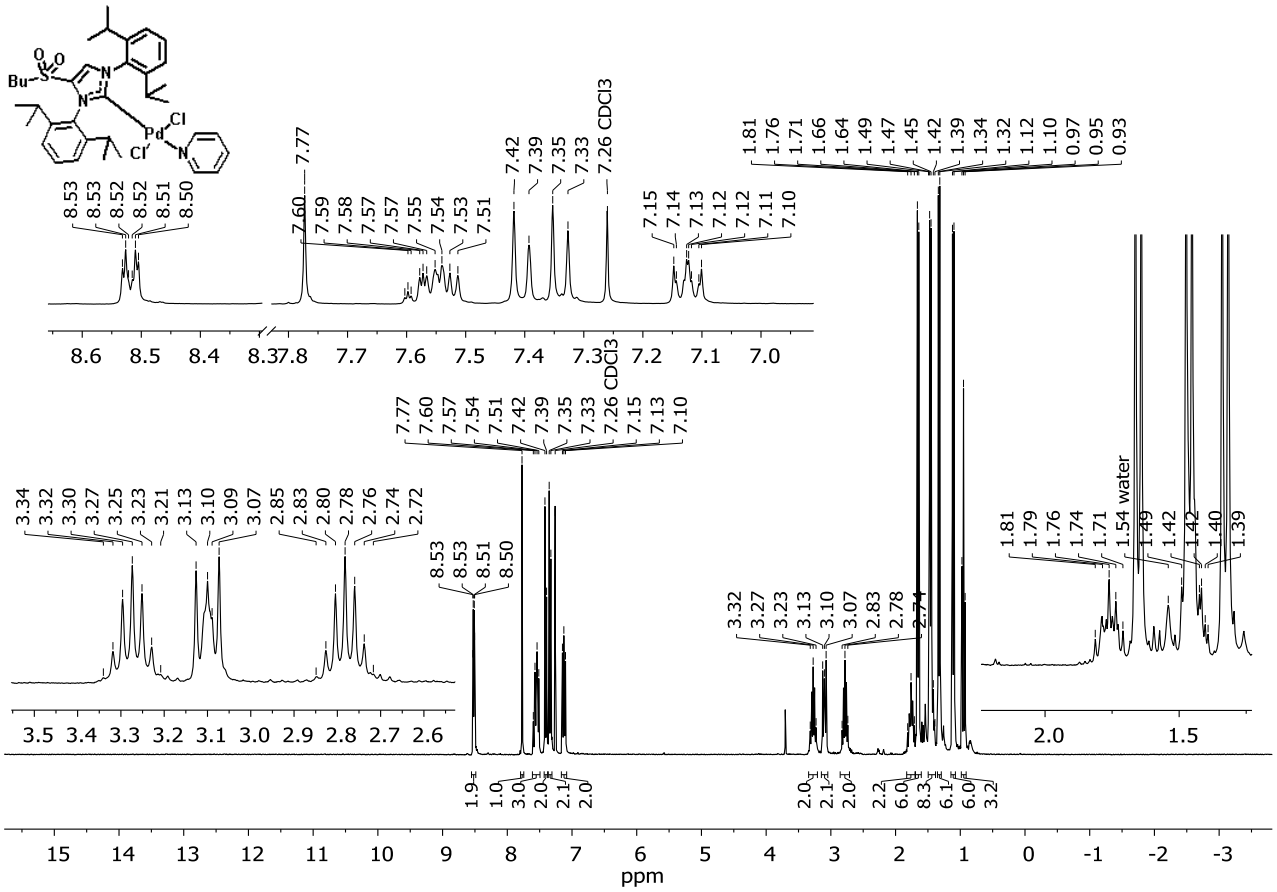


Figure S43. ^{1}H NMR spectrum of **3e** ($CDCl_3$, 300 MHz)

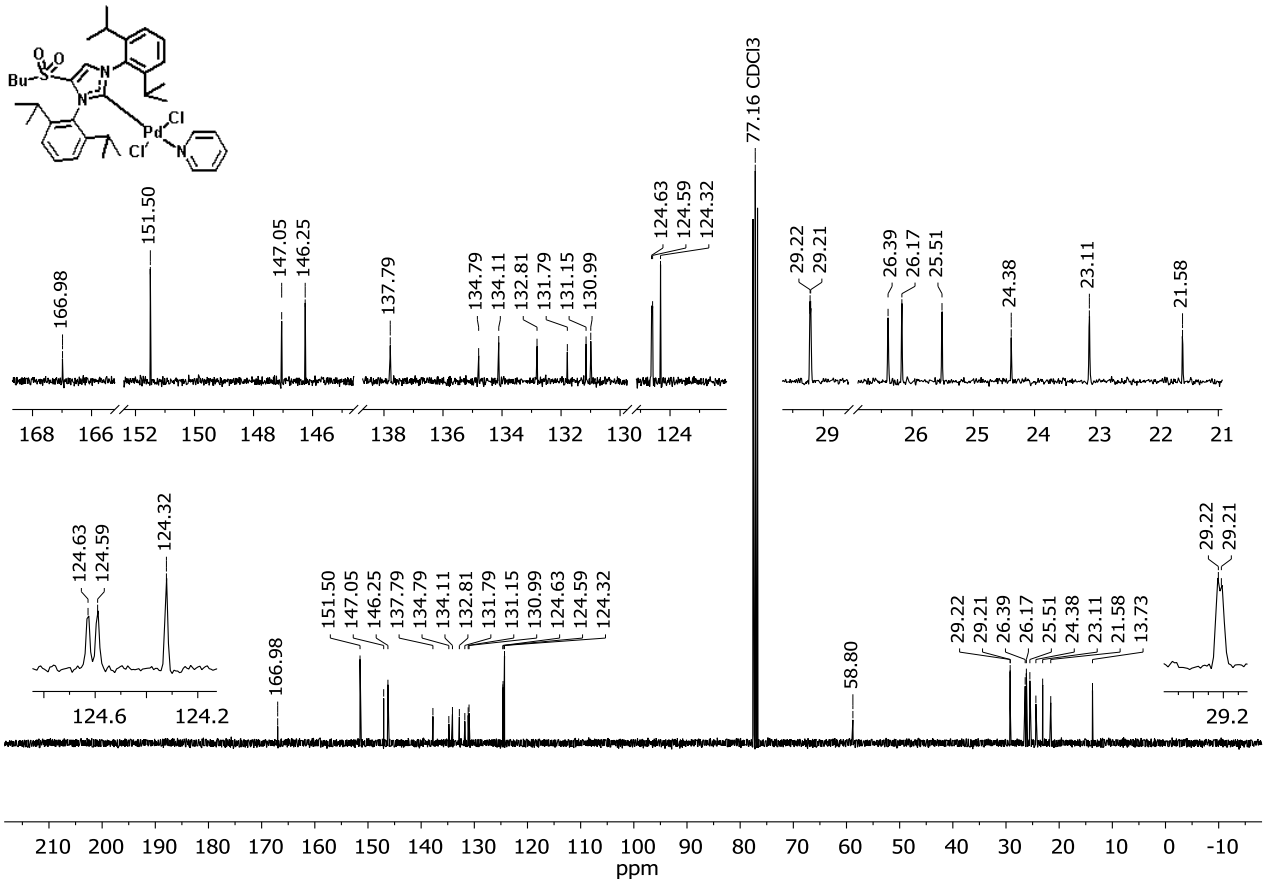


Figure S44. ^{13}C NMR spectrum of **3e** ($CDCl_3$, 75 MHz)

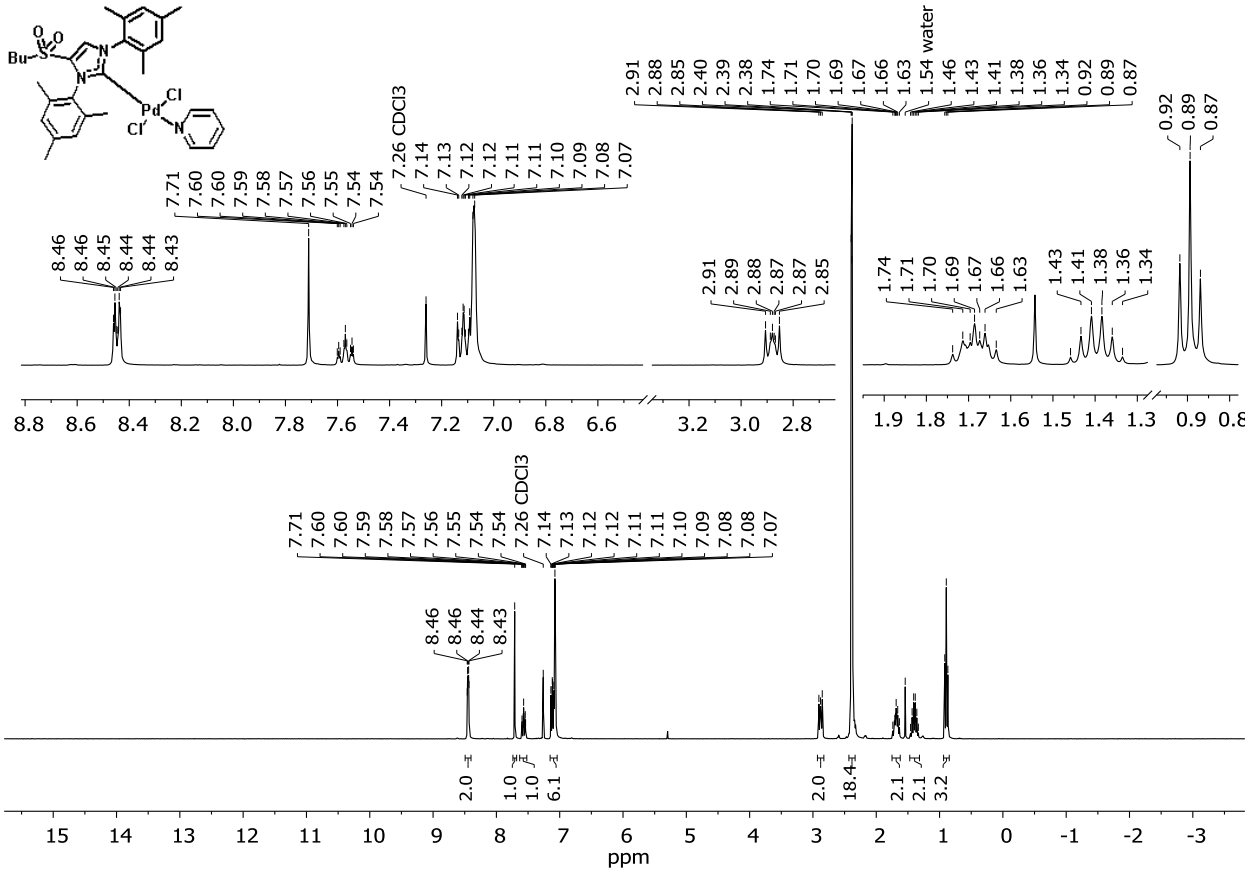


Figure S45. ^{1}H NMR spectrum of **3f** ($CDCl_3$, 300 MHz)

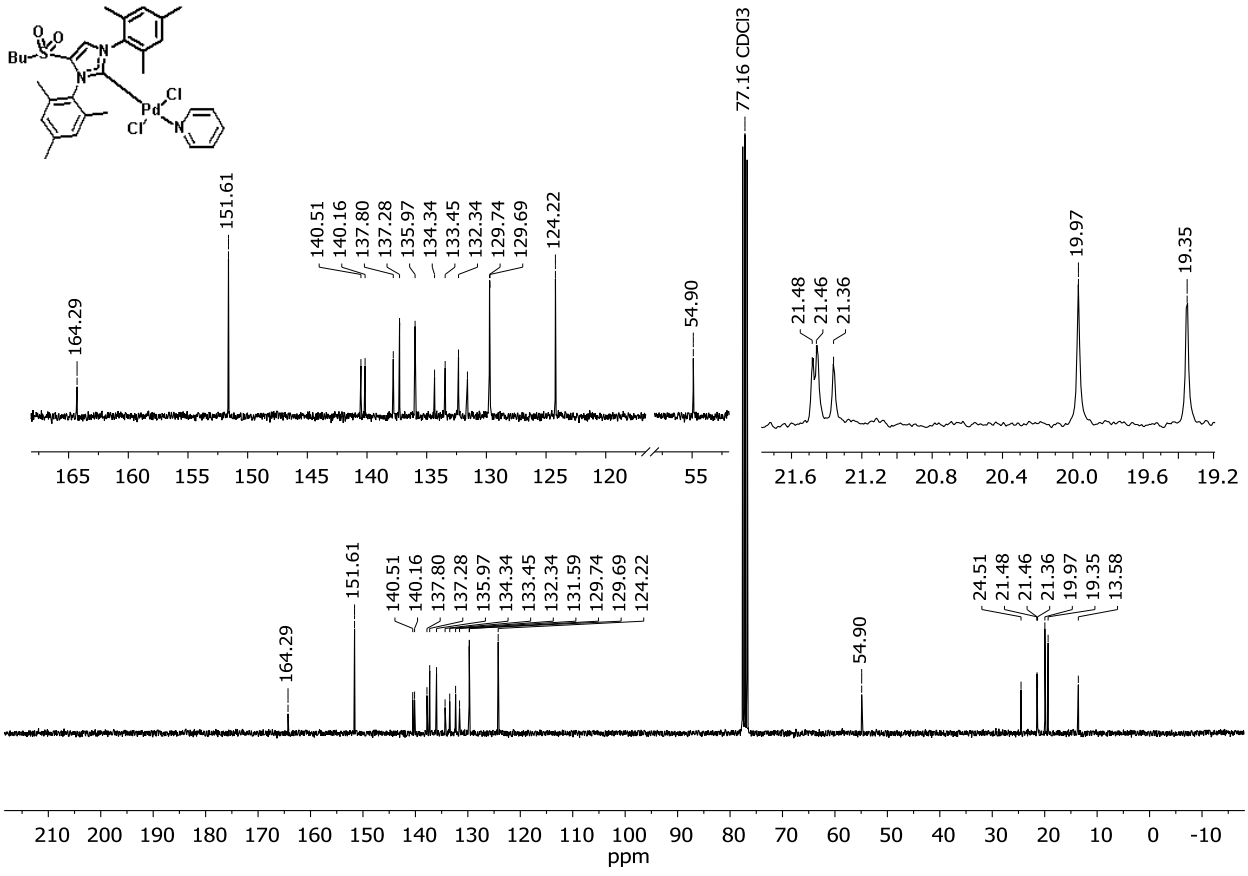


Figure S46. ^{13}C NMR spectrum of **3f** ($CDCl_3$, 75 MHz)

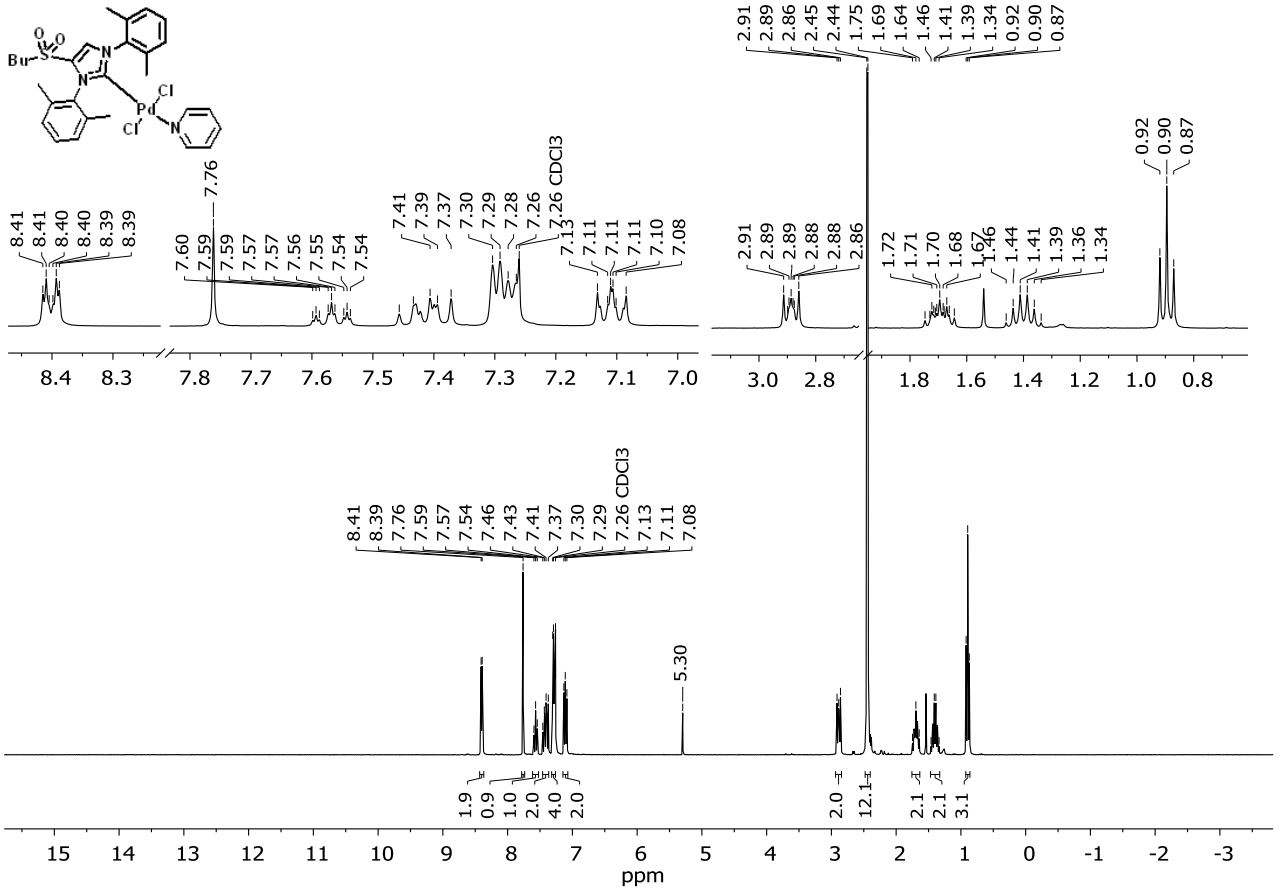


Figure S47. ^{1}H NMR spectrum of **3g** ($CDCl_3$, 300 MHz)

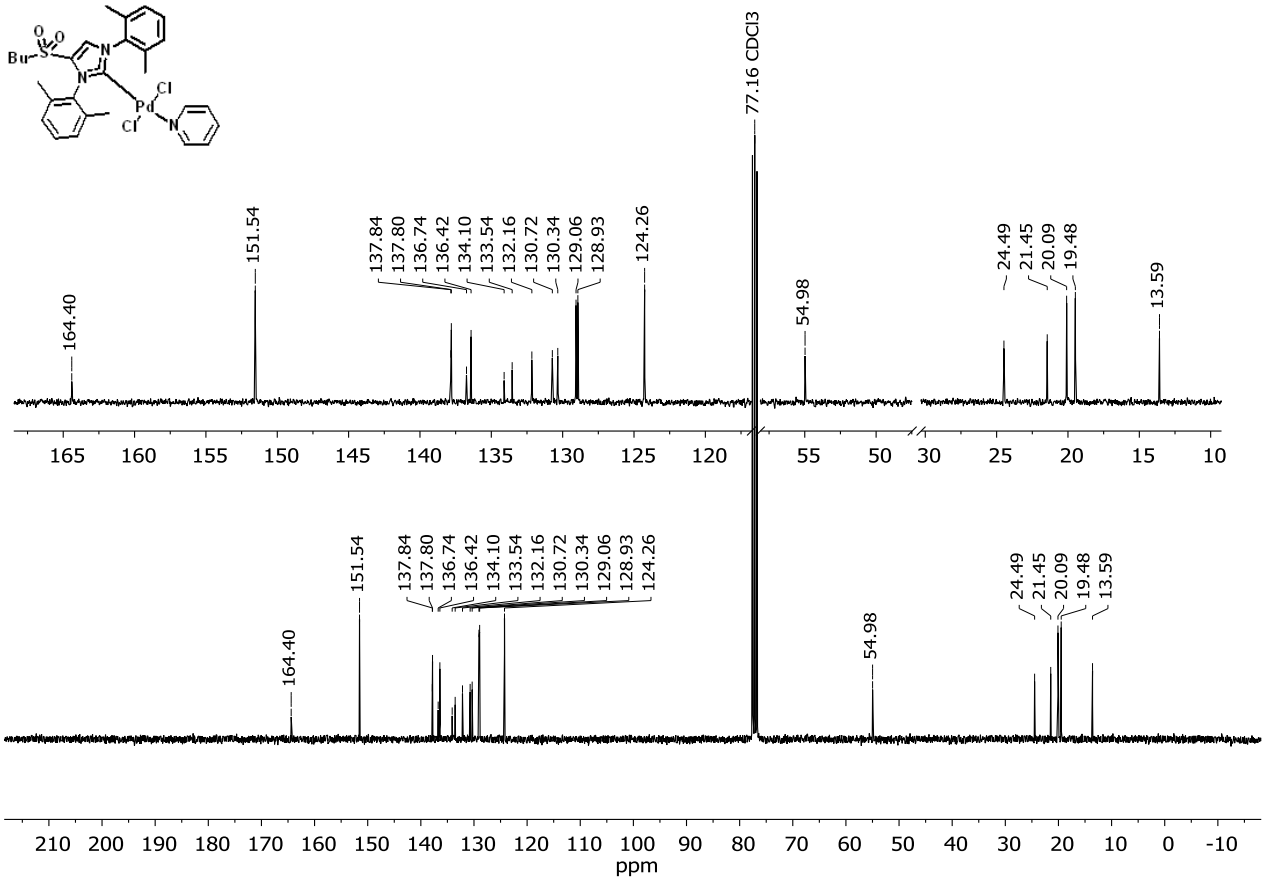


Figure S48. ^{13}C NMR spectrum of **3g** ($CDCl_3$, 75 MHz)

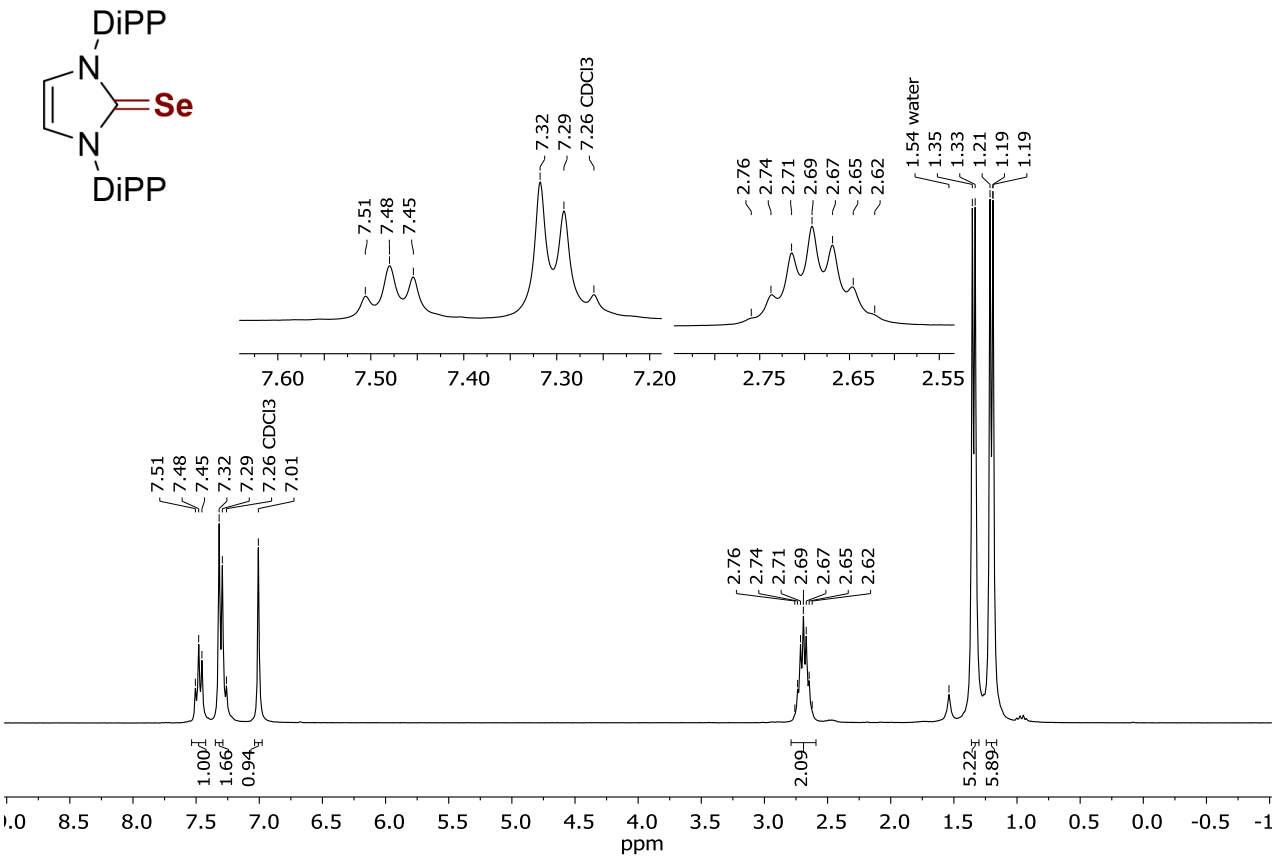


Figure S49. ^{1}H NMR spectrum of **8a** ($CDCl_3$, 300 MHz)

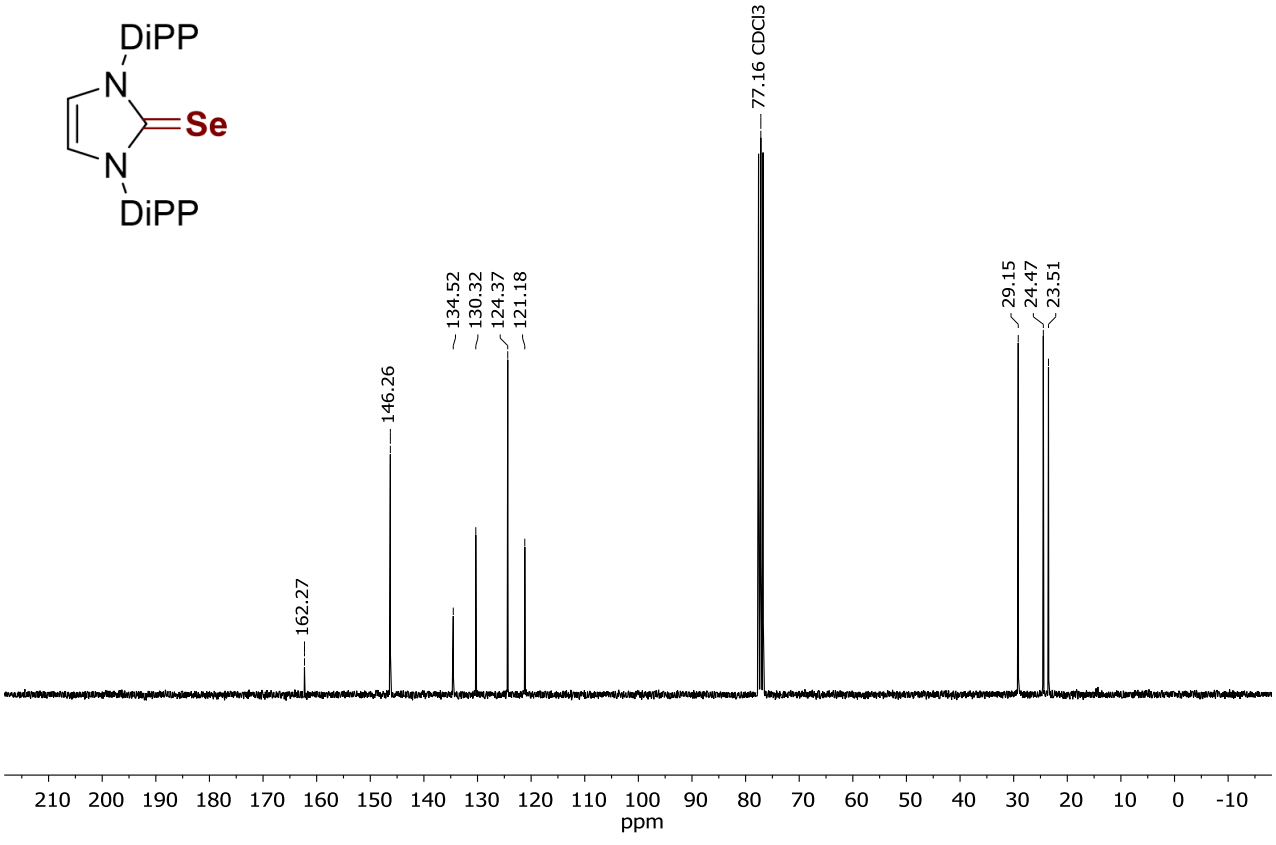


Figure S50. ^{13}C NMR spectrum of **8a** ($CDCl_3$, 75 MHz)

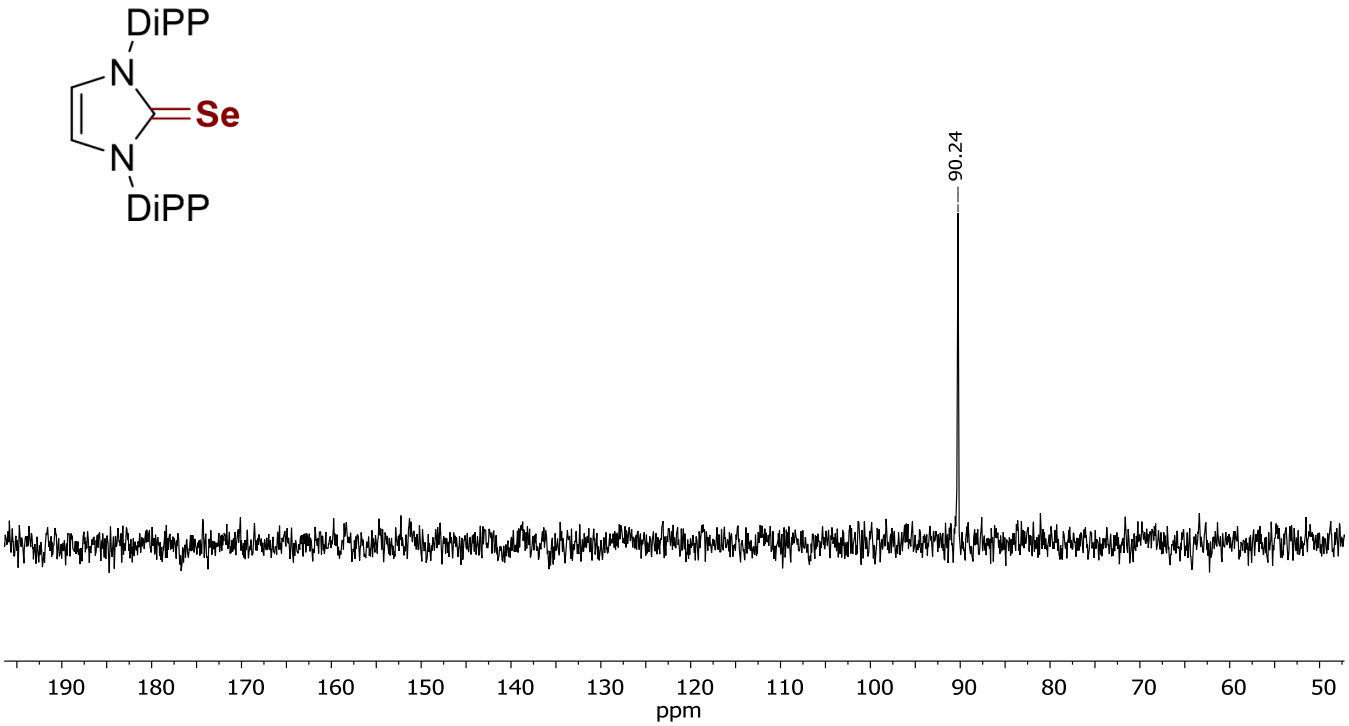


Figure S51. ^{77}Se NMR spectrum of **8a** ($CDCl_3$, 57 MHz)

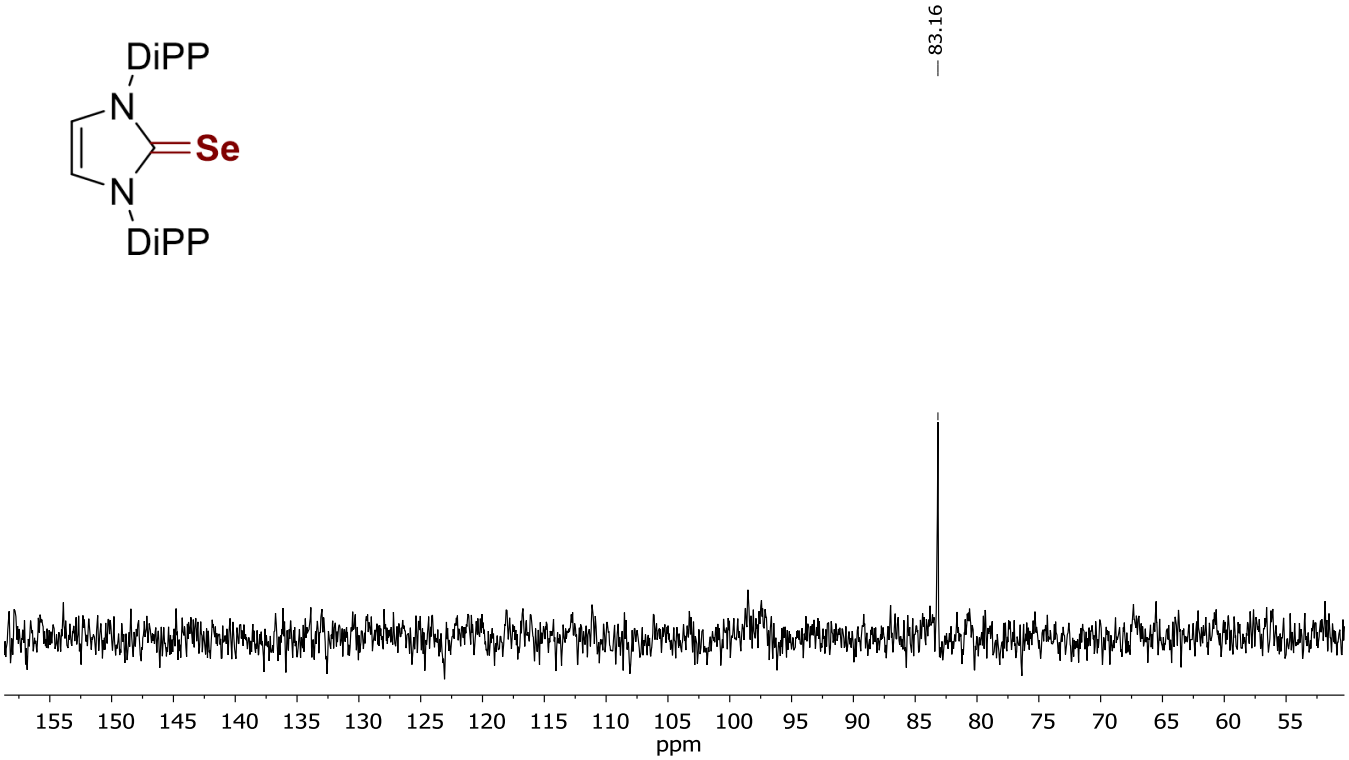


Figure S52. ^{77}Se NMR spectrum of **8a** (DMSO-d_6, 57 MHz)

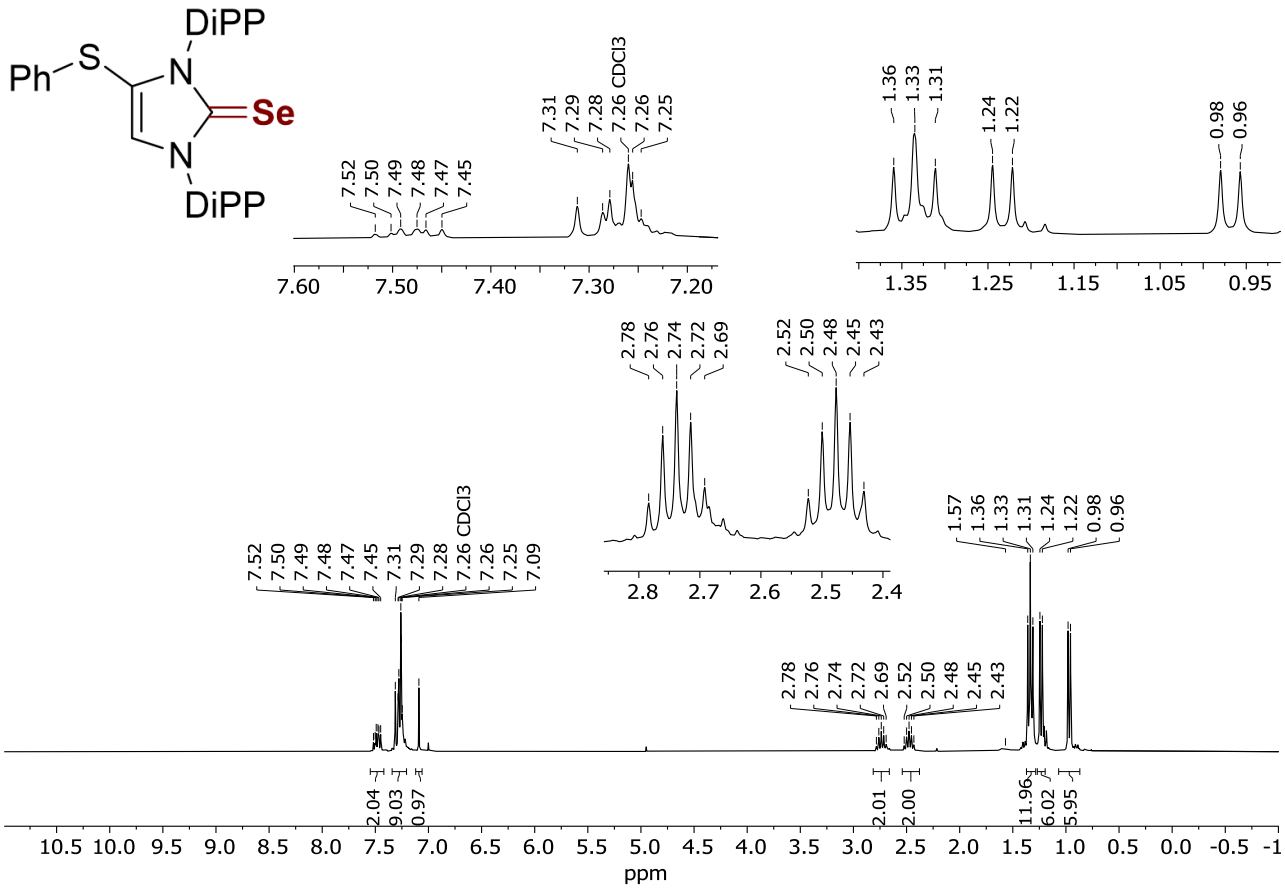


Figure S53. ^{1}H NMR spectrum of **8b** ($CDCl_3$, 300 MHz)

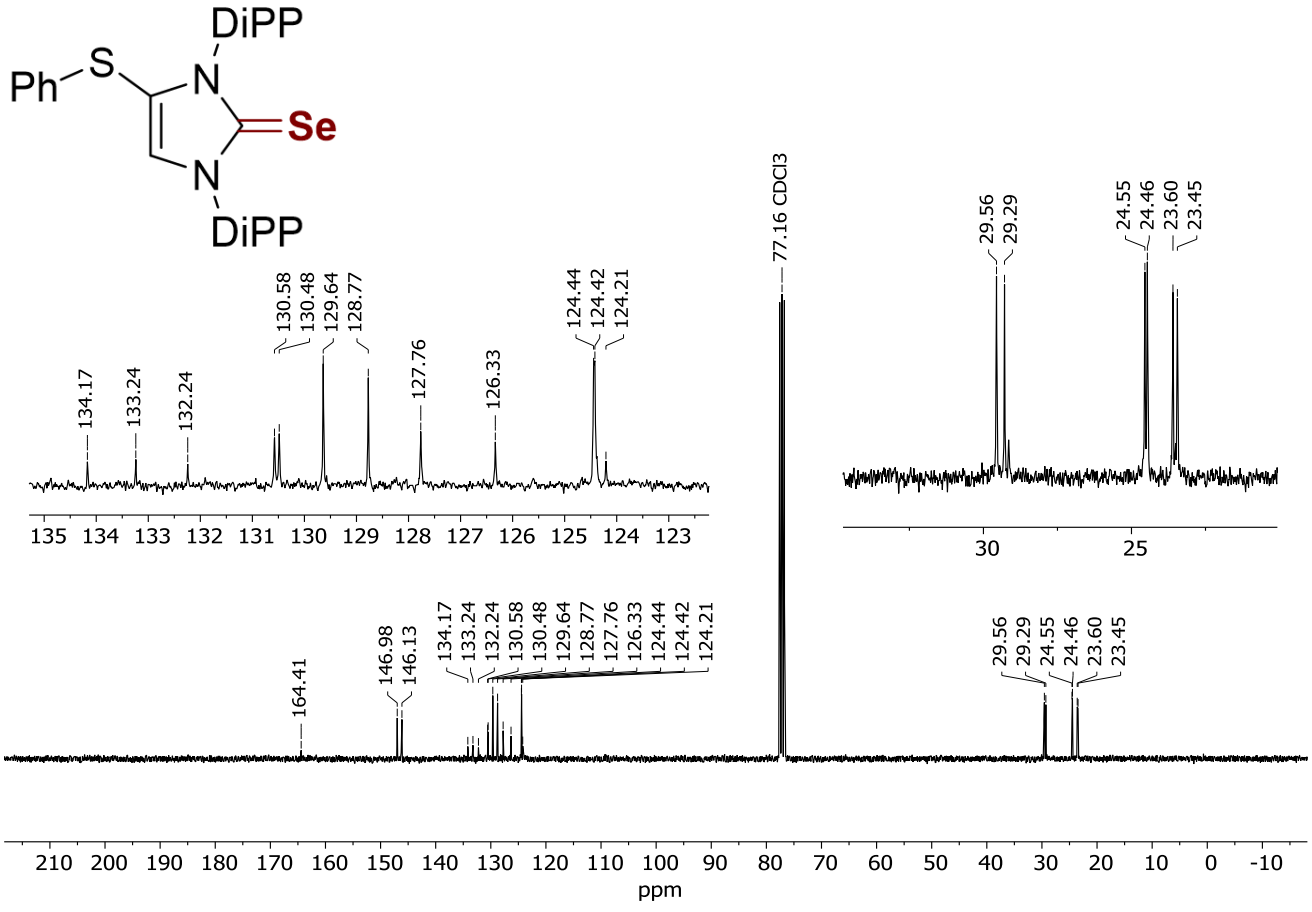


Figure S54. ^{13}C NMR spectrum of **8b** ($CDCl_3$, 75 MHz)

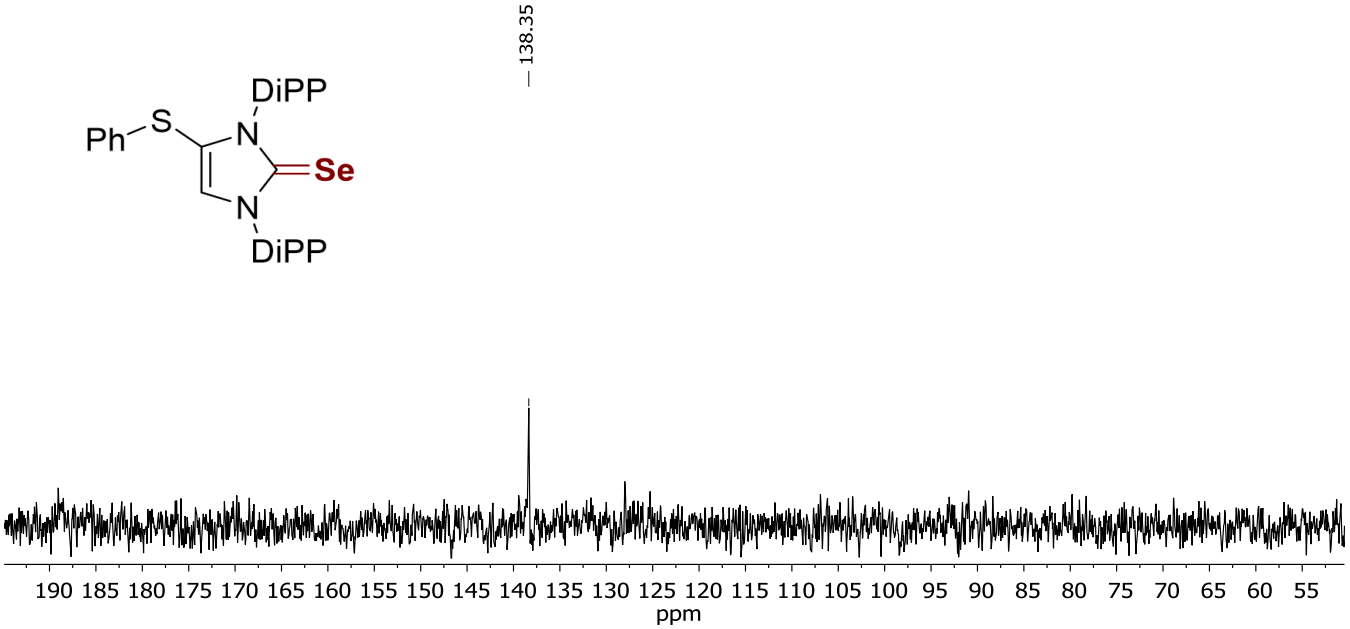


Figure S55. ^{77}Se NMR spectrum of **8b** ($CDCl_3$, 57 MHz)

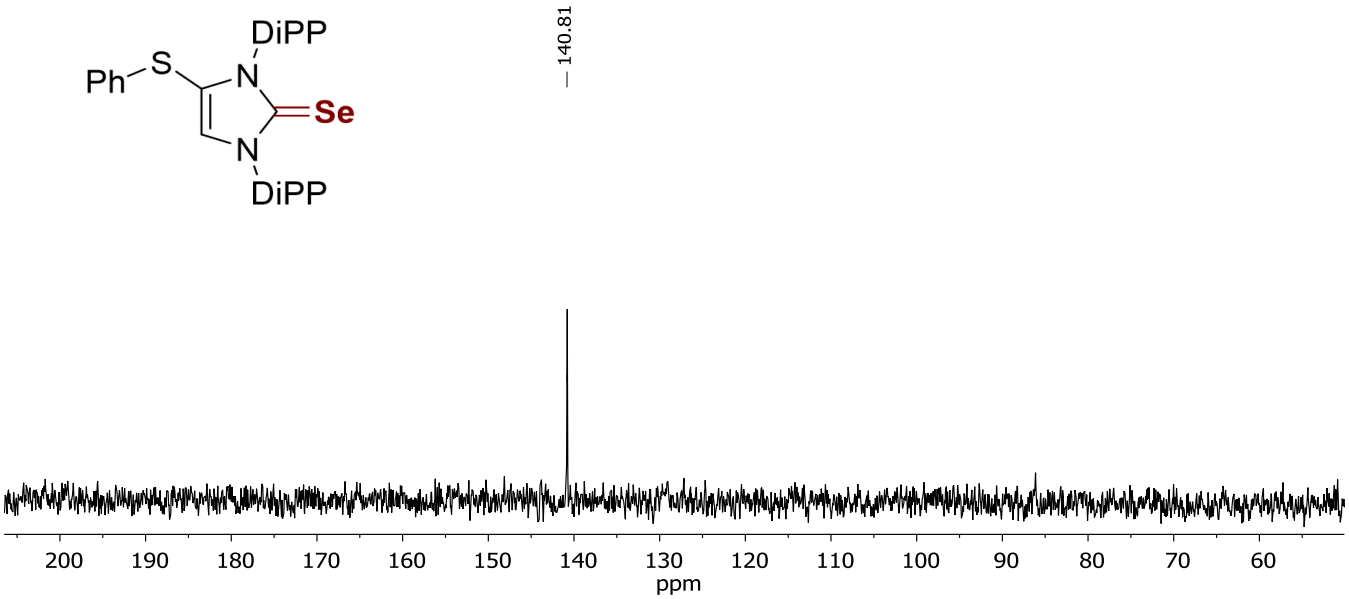


Figure S56. ^{77}Se NMR spectrum of **8b** (DMSO-d_6, 57 MHz)

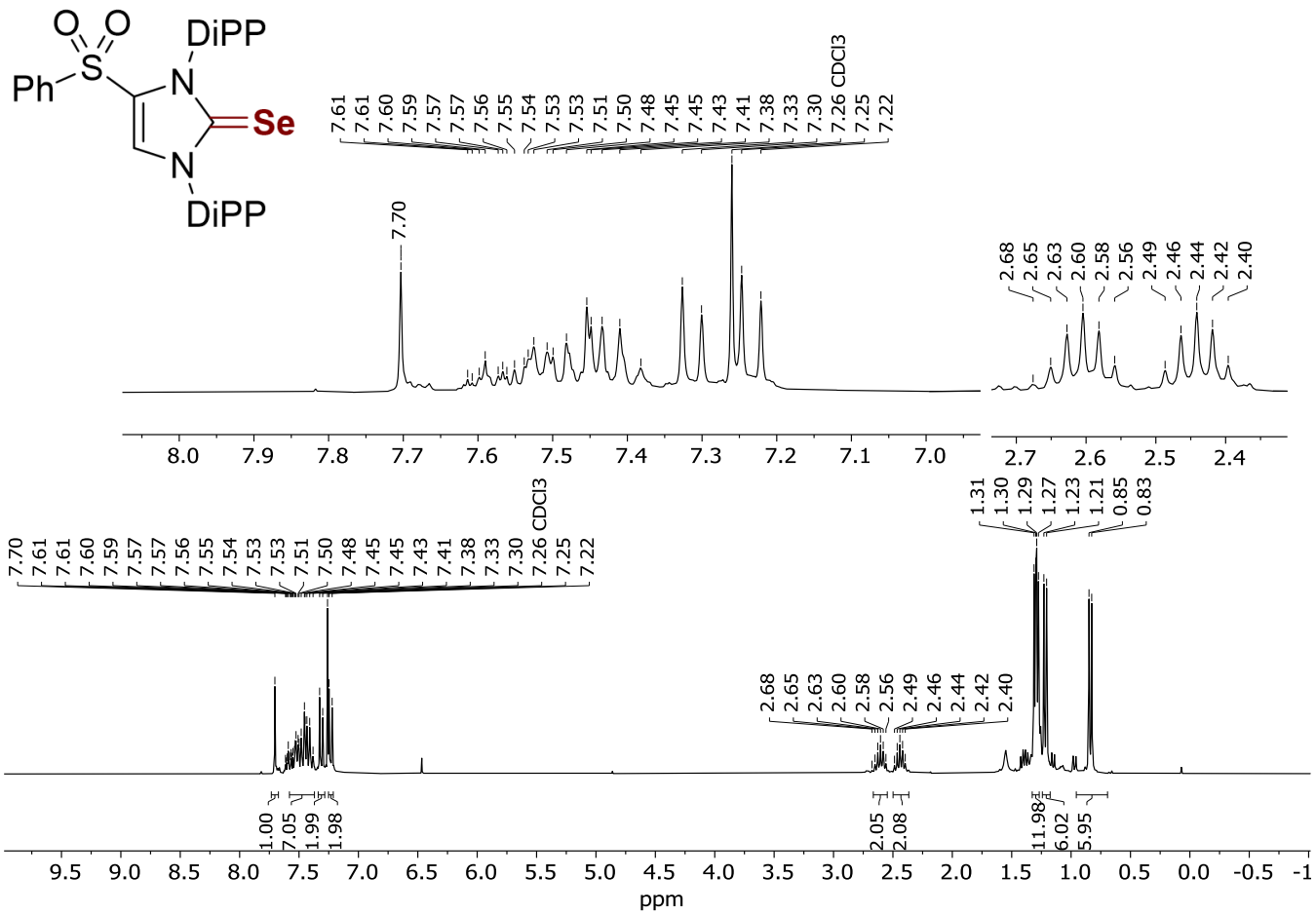


Figure S57. ^{1}H NMR spectrum of **8c** ($CDCl_3$, 300 MHz)

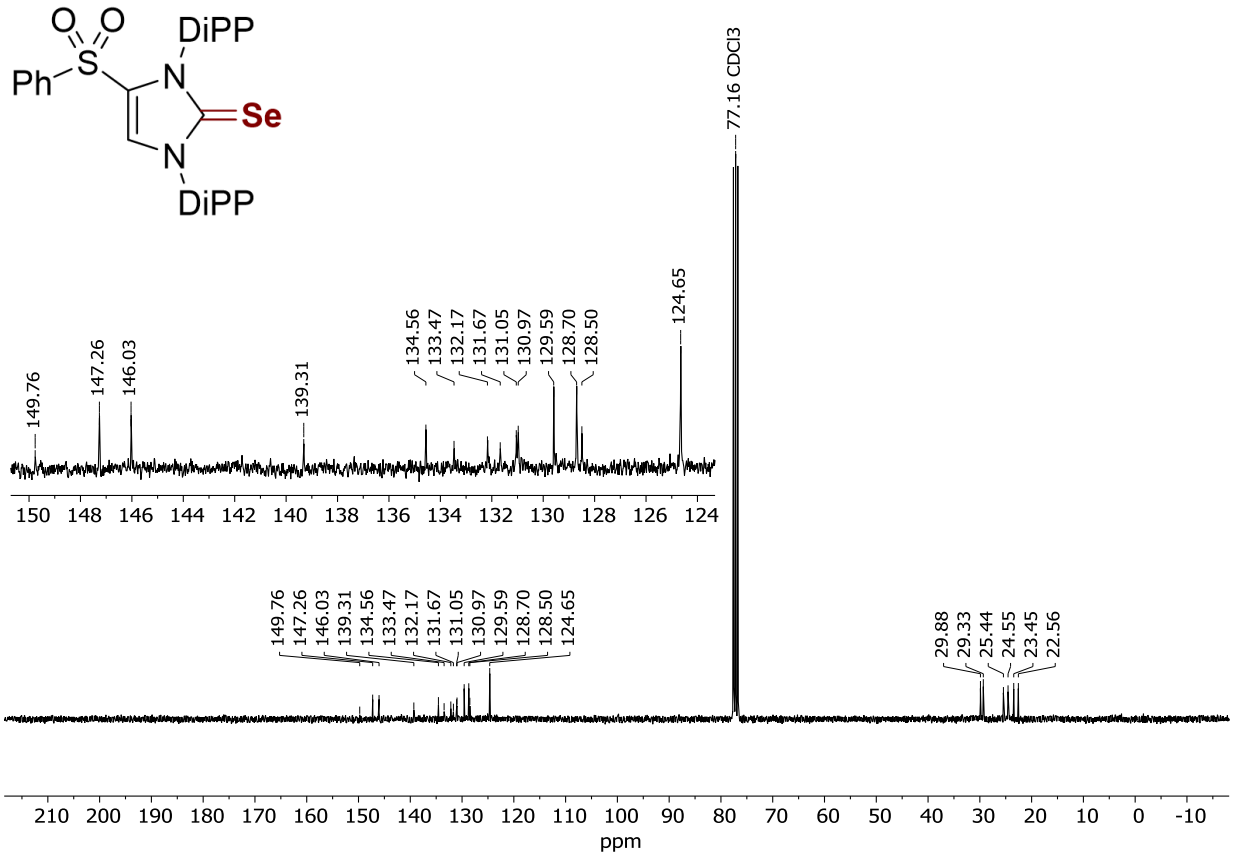


Figure S58. ^{13}C NMR spectrum of **8c** ($CDCl_3$, 75 MHz)

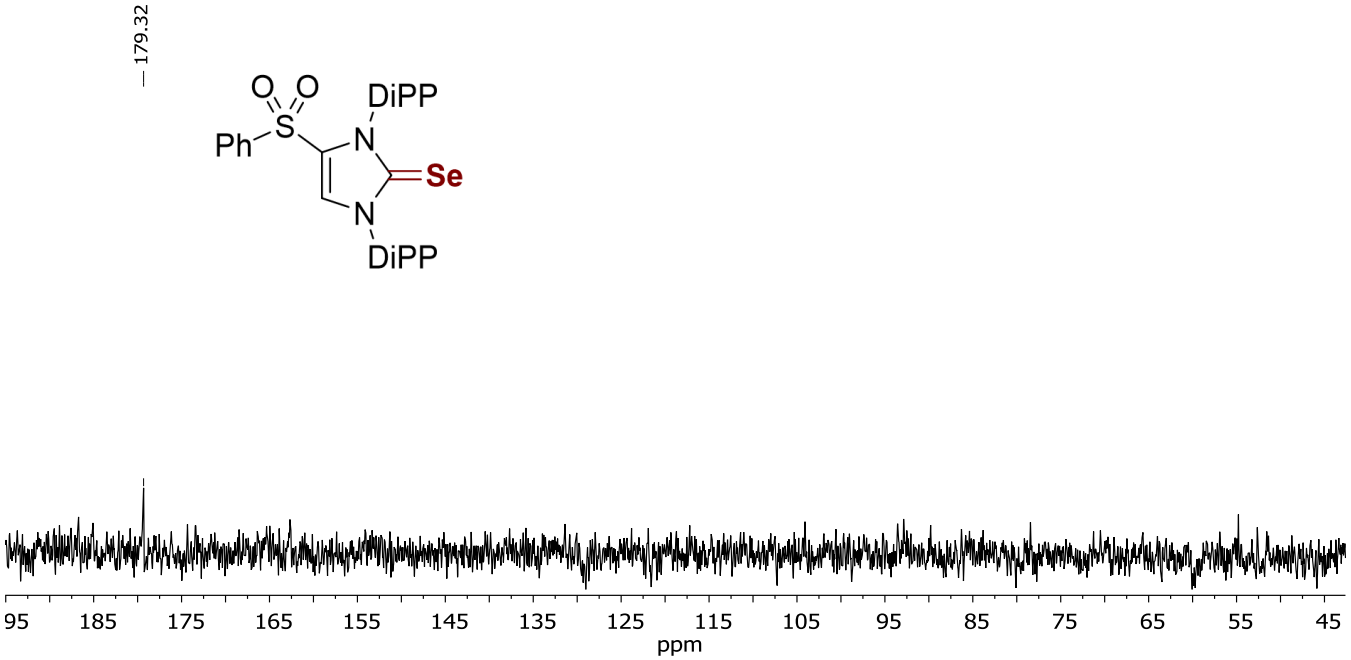


Figure S59. ^{77}Se NMR spectrum of **8c** ($CDCl_3$, 57 MHz)

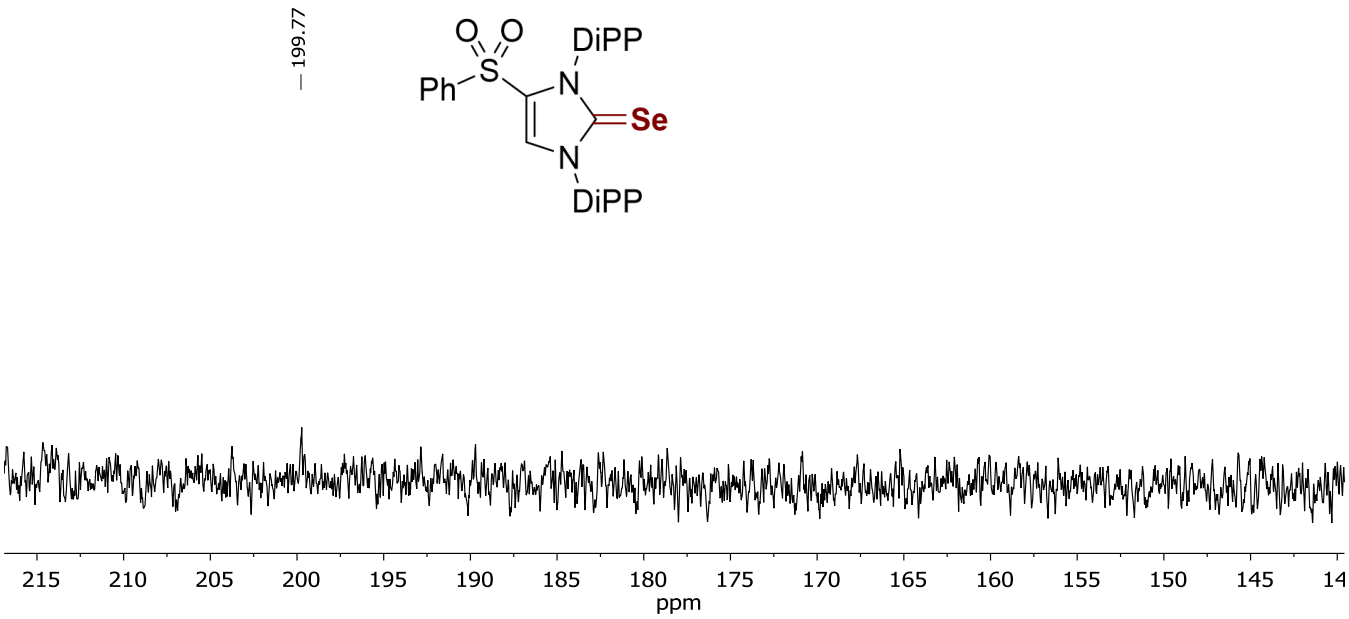


Figure S60. ^{77}Se NMR spectrum of **8c** (DMSO-d_6, 57 MHz)

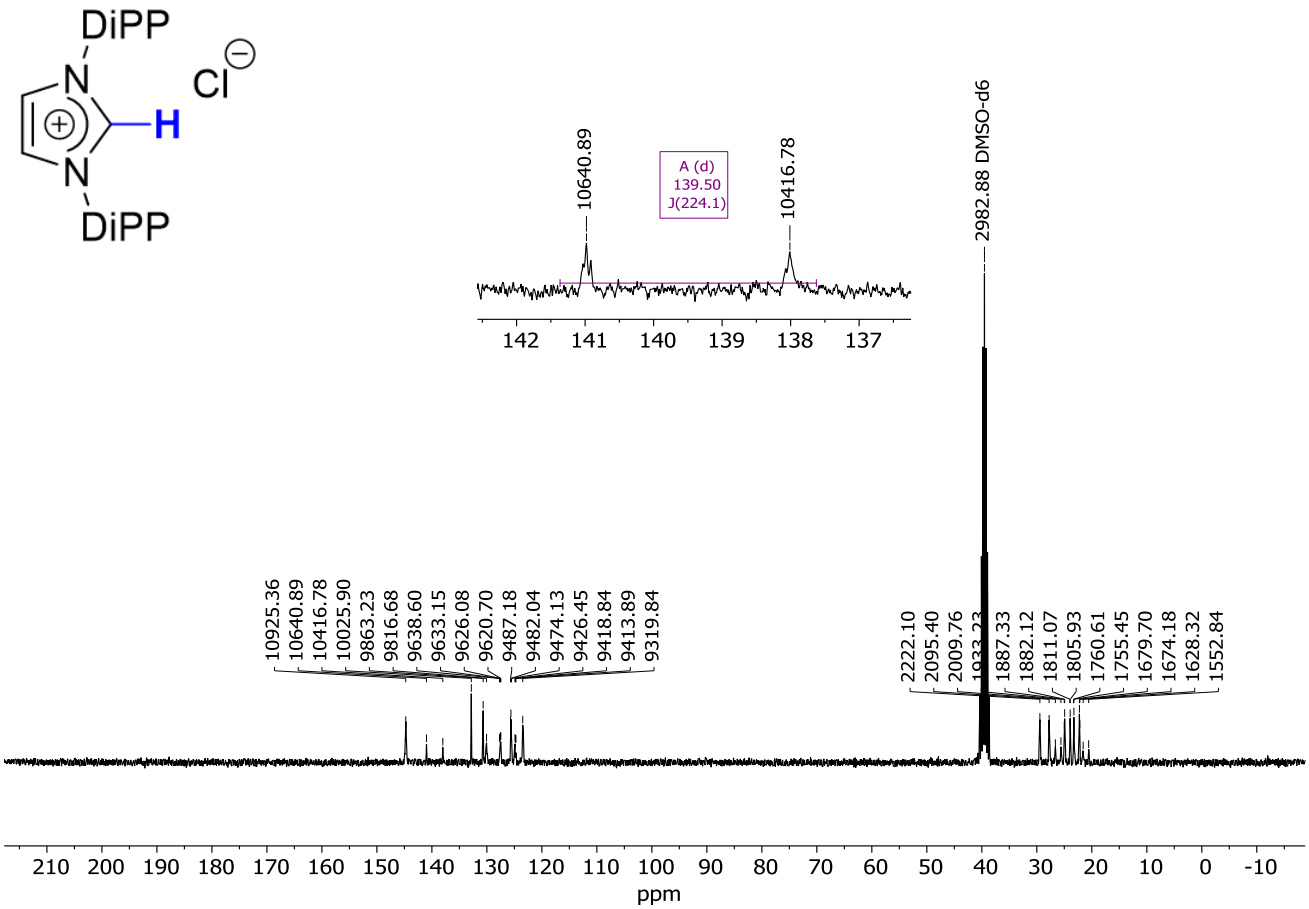


Figure S61. Non ^{1}H-decoupled ^{13}C NMR spectrum of **IPr•HCl** ($CDCl_3$, 75 MHz)

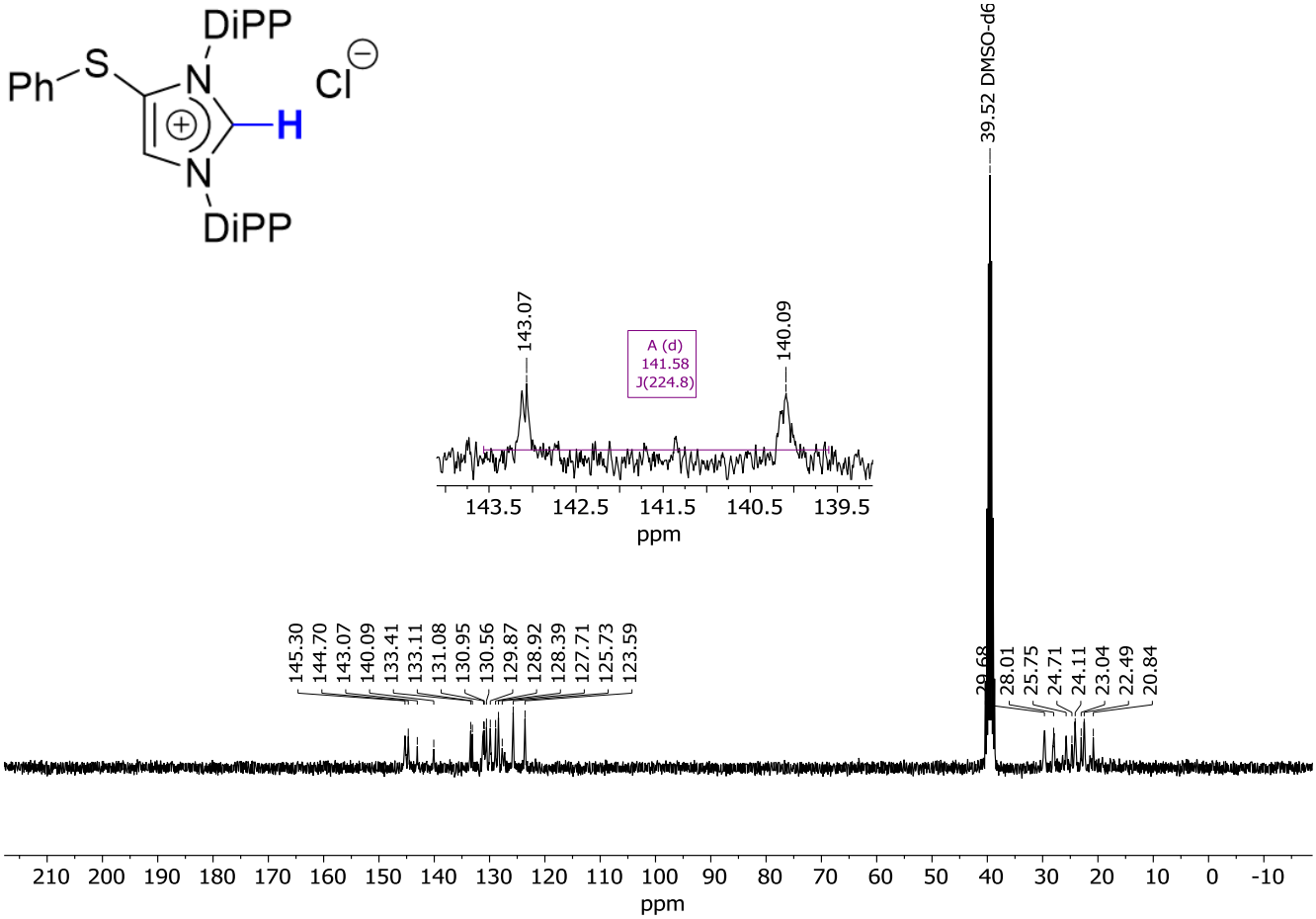


Figure S62. Non ^{1}H decoupled ^{13}C NMR spectrum of **1b** ($CDCl_3$, 75 MHz)

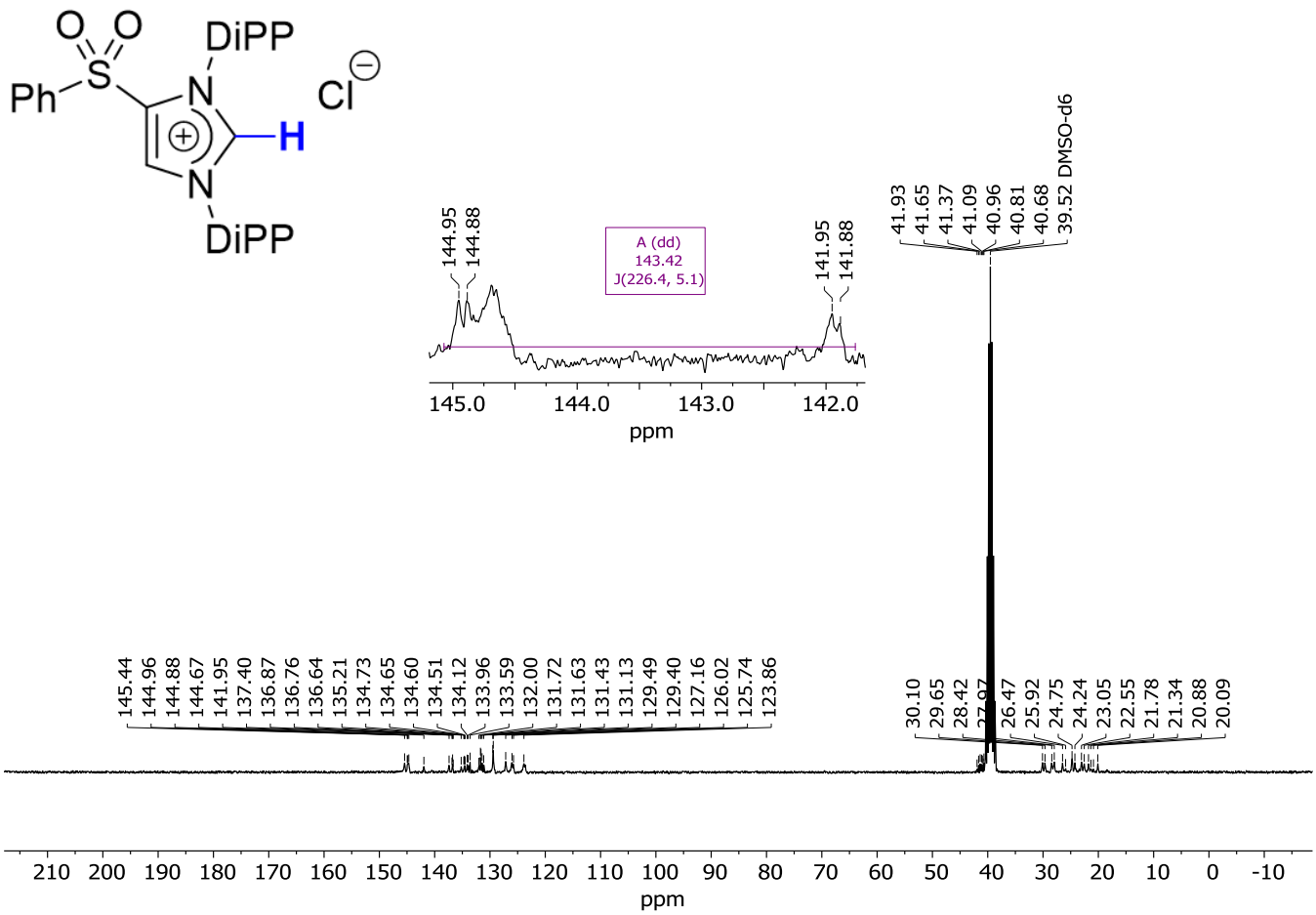


Figure S63. Non ^{1}H decoupled ^{13}C NMR spectrum of **2b** ($CDCl_3$, 75 MHz)

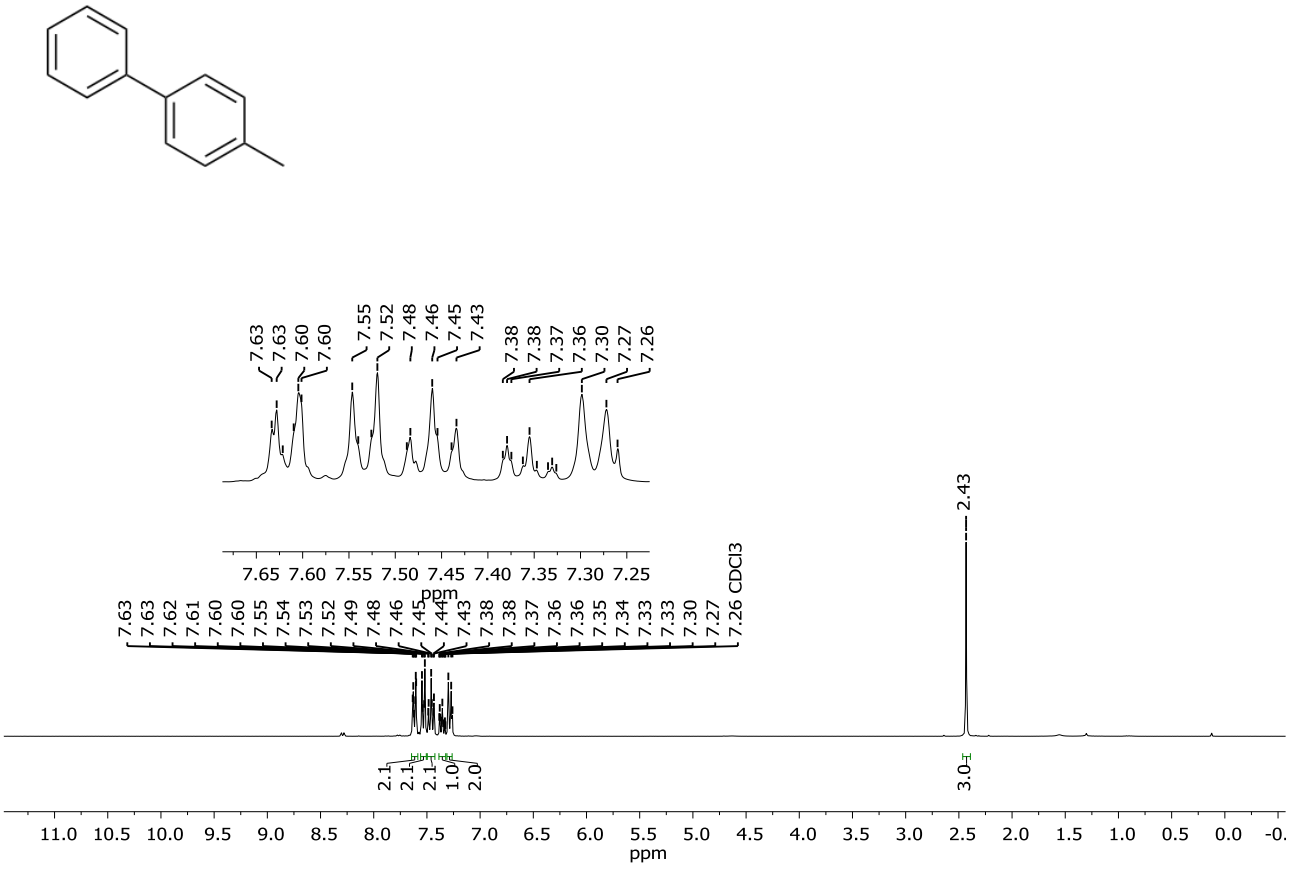


Figure S64. ^{1}H NMR spectrum of **12** ($CDCl_3$, 300 MHz)

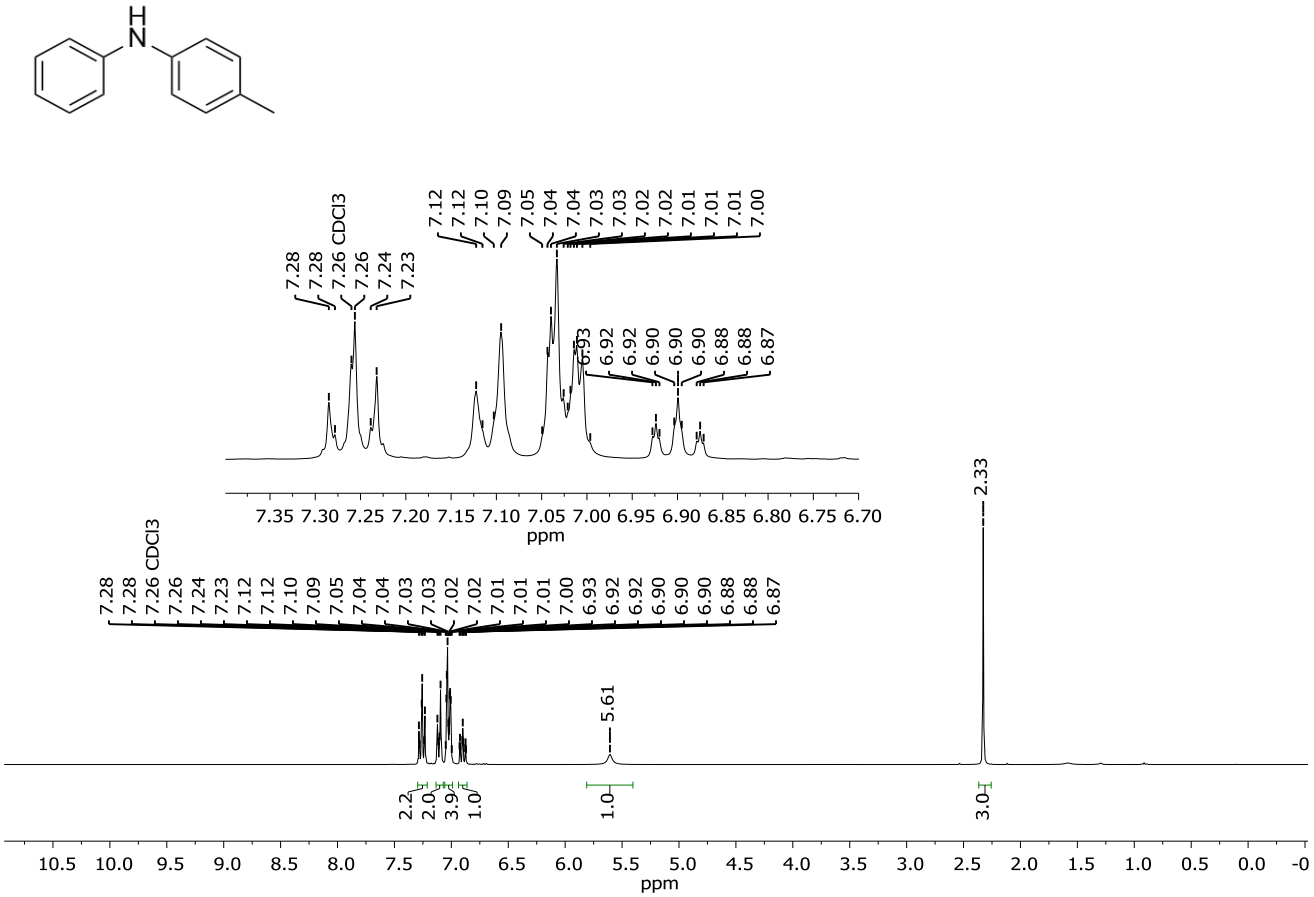


Figure S65. ^{1}H NMR spectrum of **14** ($CDCl_3$, 300 MHz)

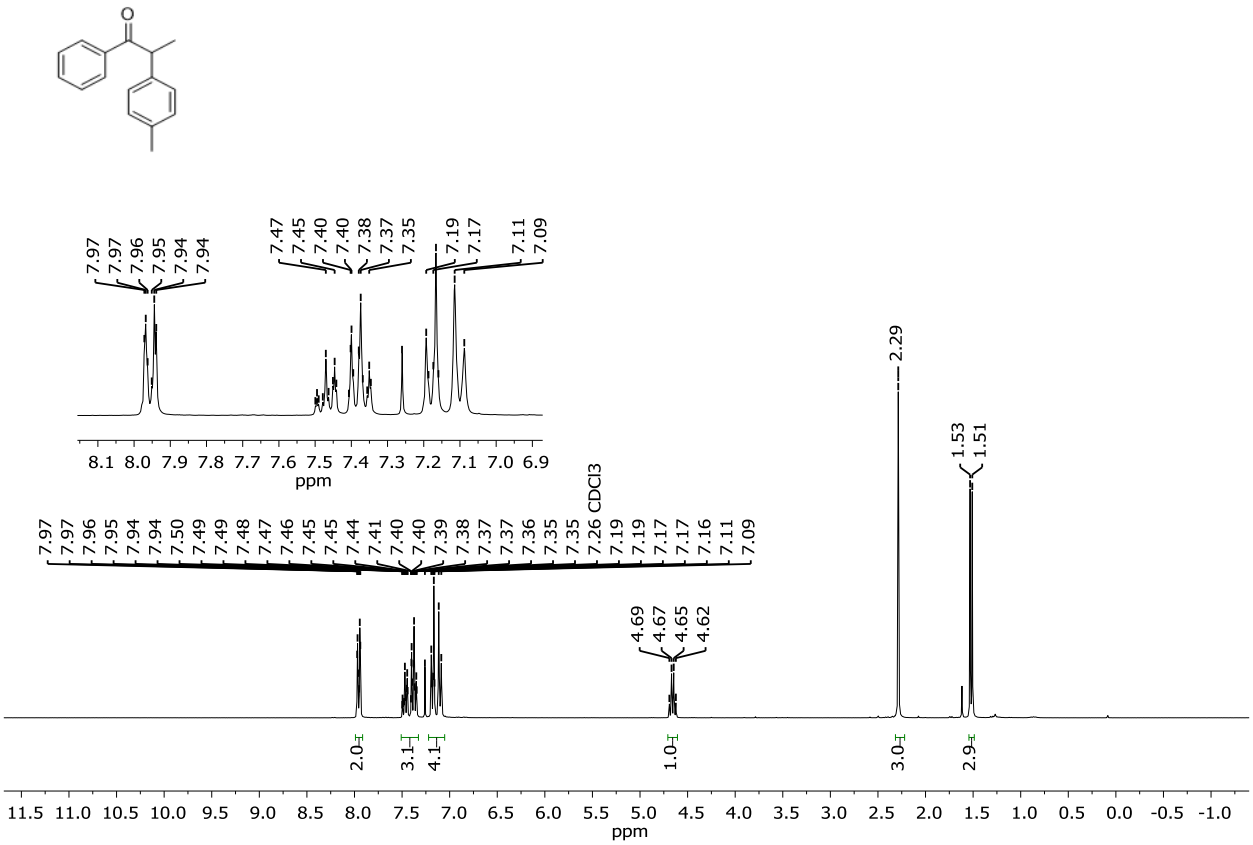
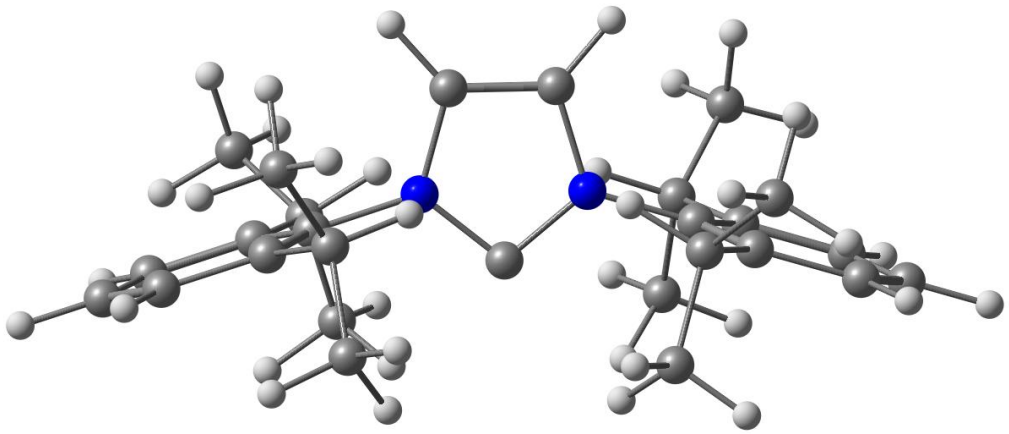


Figure S66. ^{1}H NMR spectrum of **17** ($CDCl_3$, 300 MHz)

S5. Cartesian coordinates of DFT optimized structures

Coordinates of the optimized structure of **IPr**



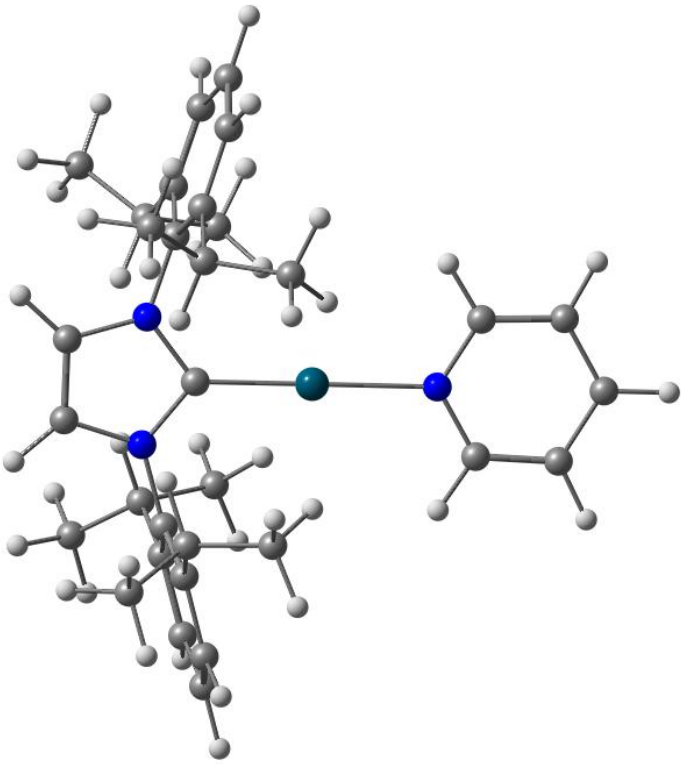
65

IPr E = -1159.0377755

C	0.6773420	-0.0337000	1.8510090
C	-0.6771940	0.0327890	1.8510970
N	1.0583110	-0.0526600	0.5172580
N	-1.0583020	0.0524340	0.5174000
C	-0.0000410	0.0001120	-0.3410620
C	2.4233310	-0.1123410	0.0927650
C	-2.4233480	0.1123130	0.0930290
C	-3.0101390	1.3717990	-0.1352640
C	-4.3475810	1.4034410	-0.5432560
C	-5.0750100	0.2290370	-0.7123130
C	-4.4740520	-1.0029290	-0.4782920
C	-3.1378500	-1.0885040	-0.0712120
C	-2.4989720	-2.4467660	0.1528580
C	-2.2155290	2.6581270	-0.0037930
C	3.1376390	1.0885660	-0.0715890
C	4.4738420	1.0031660	-0.4787210
C	5.0749950	-0.2287230	-0.7126160
C	4.3477580	-1.4032330	-0.5434310
C	3.0103120	-1.3717630	-0.1354590
C	2.2158060	-2.6581610	-0.0040580
C	2.4986020	2.4467490	0.1525010
H	-4.8286500	2.3653260	-0.7352420
H	-5.0529560	-1.9197220	-0.6173030
H	-1.4738810	-2.2750290	0.5131210
C	-3.2330770	-3.2527930	1.2251990
C	-2.3903590	-3.2239530	-1.1606990
H	-1.3080120	2.4266330	0.5747180
H	5.0525950	1.9200390	-0.6178270
H	4.8289820	-2.3650560	-0.7353270
H	1.3084770	-2.4268700	0.5748350
C	1.7624270	-3.1417940	-1.3844970
C	2.9711950	-3.7503130	0.7515340
H	1.4735460	2.2748810	0.5128000

H	-1.3922880	0.0665930	2.6692150
H	1.3925260	-0.0678900	2.6690320
H	-6.1193610	0.2753320	-1.0313890
H	6.1193520	-0.2748840	-1.0316930
C	-2.9706710	3.7500320	0.7524190
C	-1.7625850	3.1421680	-1.3842200
C	3.2326550	3.2528570	1.2248190
C	2.3898510	3.2239360	-1.1610440
H	-2.7173190	-4.2085750	1.4082190
H	-3.2800930	-2.7046440	2.1787360
H	-4.2658690	-3.4881260	0.9223150
H	-1.8745950	-4.1839970	-1.0000640
H	-3.3843710	-3.4450390	-1.5819380
H	-1.8235540	-2.6532160	-1.9113350
H	1.1430300	-4.0486390	-1.2950890
H	1.1691610	-2.3683810	-1.8946590
H	2.6292040	-3.3848000	-2.0204780
H	2.3194200	-4.6241370	0.9063580
H	3.8554120	-4.1009040	0.1961620
H	3.3100650	-3.4000290	1.7385940
H	-2.3189020	4.6238700	0.9071940
H	-3.8551690	4.1006810	0.1975320
H	-3.3090720	3.3994460	1.7395320
H	-1.1432090	4.0490190	-1.2947410
H	-1.1694100	2.3689150	-1.8947320
H	-2.6295340	3.3853040	-2.0199180
H	2.7167890	4.2085750	1.4078640
H	3.2797740	2.7047080	2.1783520
H	4.2654060	3.4883150	0.9218950
H	1.8739900	4.1839220	-1.0003800
H	3.3838230	3.4451350	-1.5823180
H	1.8230790	2.6531450	-1.9116620

Coordinates of the optimized structure of **9a**



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9a E=-1535.0941195

Pd	-0.0033470	1.1668640	-0.0974120
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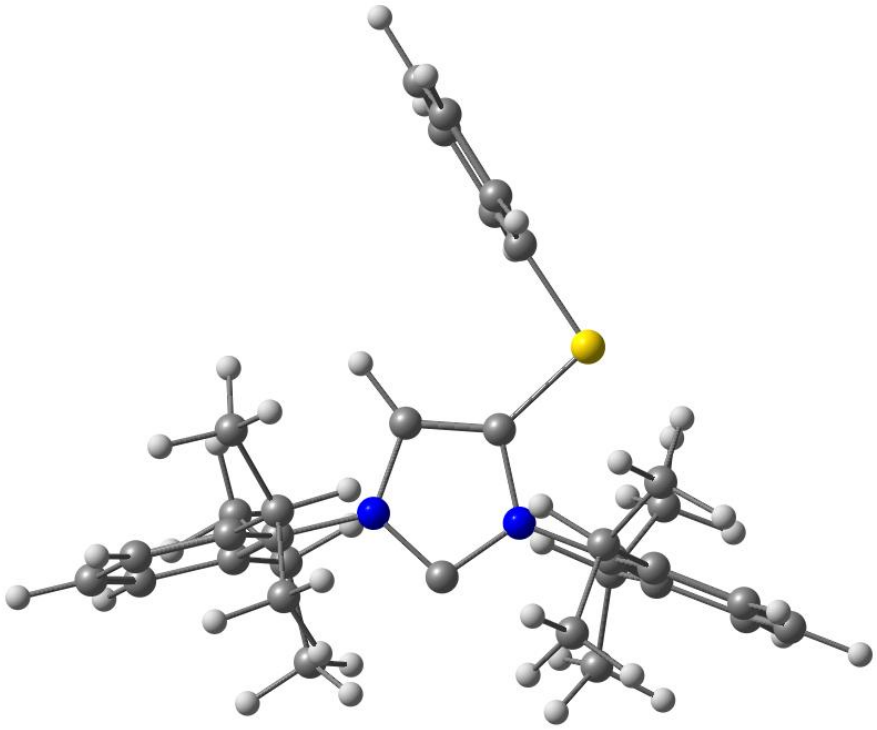
C	1.1489360	3.9506720	-0.2838280
C	-1.1533910	3.9526570	-0.2945500
C	1.1957000	5.3379630	-0.3740000
C	-1.1969450	5.3400330	-0.3851350
C	0.0001970	6.0510030	-0.4256440
H	2.0647280	3.3571170	-0.2409770
H	-2.0707100	3.3609660	-0.2602000
H	2.1621110	5.8446380	-0.4027290
H	-2.1621990	5.8483340	-0.4228850
H	0.0014600	7.1413640	-0.4964530
C	0.6789220	-2.9596790	0.2691620
C	-0.6767450	-2.9613280	0.2678650
N	1.0702940	-1.6383170	0.1377030
N	-1.0708870	-1.6409460	0.1350880
C	-0.0013480	-0.7890450	0.0531230
C	2.4368530	-1.2190860	0.0996300
C	-2.4377660	-1.2246730	0.0841780
C	-3.0882440	-0.8744280	1.2824340
C	-4.4296670	-0.4851650	1.2042980
C	-5.0973010	-0.4475800	-0.0156090
C	-4.4332870	-0.8039070	-1.1851020
C	-3.0926530	-1.2026210	-1.1615840
C	-2.3834230	-1.5603020	-2.4552060
C	-2.3819900	-0.8962170	2.6251710
C	3.0904970	-0.9227010	1.3105840
C	4.4318290	-0.5306810	1.2474340
C	5.0970990	-0.4395630	0.0290410

C	4.4304730	-0.7442310	-1.1534740
C	3.0898050	-1.1434270	-1.1450000
C	2.3812720	-1.4503980	-2.4517180
C	2.3840290	-0.9953260	2.6513990
H	-4.9602030	-0.2027220	2.1174700
H	-4.9663120	-0.7683580	-2.1385200
H	-1.3919590	-1.9577860	-2.1908870
C	-3.1188870	-2.6517670	-3.2334460
C	-2.1529970	-0.3120820	-3.3096390
H	-1.3546610	-1.2503050	2.4530020
H	4.9637730	-0.2881880	2.1711900
H	4.9616770	-0.6682300	-2.1056150
H	1.3802670	-1.8338620	-2.2031940
C	2.1823940	-0.1757970	-3.2740590
C	3.1006700	-2.5360510	-3.2530820
H	1.3630410	-1.3623050	2.4688490
H	-1.3907530	-3.7765140	0.3466940
H	1.3947860	-3.7730760	0.3496480
H	-6.1450120	-0.1385050	-0.0552770
H	6.1447840	-0.1291500	0.0008700
C	-3.0482830	-1.8703690	3.5981660
C	-2.2751350	0.5110350	3.2144650
C	3.0647140	-1.9829790	3.6001170
C	2.2524740	0.3945410	3.2762270
H	-2.5409510	-2.9409150	-4.1252730
H	-3.2699270	-3.5533430	-2.6198420
H	-4.1078970	-2.3124570	-3.5805500
H	-1.6016220	-0.5682980	-4.2285520
H	-3.1081970	0.1501950	-3.6074710
H	-1.5656290	0.4346440	-2.7513420
H	1.6268050	-0.3952470	-4.1998620
H	1.6107310	0.5685270	-2.6963890
H	3.1483480	0.2720960	-3.5589630
H	2.5284550	-2.7846490	-4.1607370
H	4.1024050	-2.2103750	-3.5760470
H	3.2217400	-3.4588260	-2.6648320
H	-2.4844250	-1.9162830	4.5432230
H	-4.0773870	-1.5612940	3.8421750
H	-3.0948180	-2.8881220	3.1808060
H	-1.7153230	0.4899720	4.1631470
H	-1.7453080	1.1797670	2.5170260
H	-3.2691250	0.9396910	3.4216790
H	2.5003880	-2.0618840	4.5426620
H	3.1281430	-2.9889030	3.1570850
H	4.0882450	-1.6639170	3.8541810
H	1.6889130	0.3412910	4.2214430
H	3.2390040	0.8330170	3.4982040
H	1.7163720	1.0723450	2.5929340

Coordinates of the optimized structure of **PhS-IPr**



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PhS-IPr E=-1787.95593137

C	0.9909110	-3.0550810	0.4227130
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N	1.2287080	-1.6958650	0.2509540
N	-0.8795880	-1.9212920	0.2762690
C	0.0773010	-0.9647370	0.1547910
C	2.5416500	-1.1310890	0.1814410
C	-2.2833800	-1.6502490	0.2257030
C	-2.9522660	-1.2999100	1.4141260
C	-4.3235050	-1.0350140	1.3354570
C	-5.0041840	-1.1255490	0.1250620
C	-4.3230690	-1.4832440	-1.0334410
C	-2.9503010	-1.7540950	-1.0086360
C	-2.2236660	-2.1137370	-2.2917840
C	-2.2155600	-1.1610950	2.7336180
C	3.1678040	-0.7152980	1.3714480
C	4.4509590	-0.1664840	1.2740780
C	5.0853330	-0.0387020	0.0429900
C	4.4474340	-0.4612290	-1.1191710
C	3.1658660	-1.0193700	-1.0757840
C	2.4699360	-1.4431990	-2.3556210
C	2.4917130	-0.8306000	2.7248500
H	-4.8692400	-0.7507970	2.2383070
H	-4.8674370	-1.5494650	-1.9790690
H	-1.1868900	-2.3675490	-2.0255820
C	-2.8331170	-3.3401210	-2.9715520
C	-2.1669080	-0.9130570	-3.2385200
H	-1.2433050	-1.6649830	2.6209010
H	4.9612930	0.1702040	2.1800820
H	4.9546880	-0.3534630	-2.0809590
H	1.5805720	-2.0246720	-2.0697370

C	1.9766010	-0.2162650	-3.1264280
C	3.3430470	-2.3471670	-3.2248020
H	1.5143420	-1.3100390	2.5662400
H	-0.9819160	-4.0868230	0.5514560
H	-6.0758960	-0.9146480	0.0851310
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C	-1.9298200	0.3132190	3.0307190
C	3.2885820	-1.7188050	3.6817320
C	2.2233700	0.5505480	3.3256920
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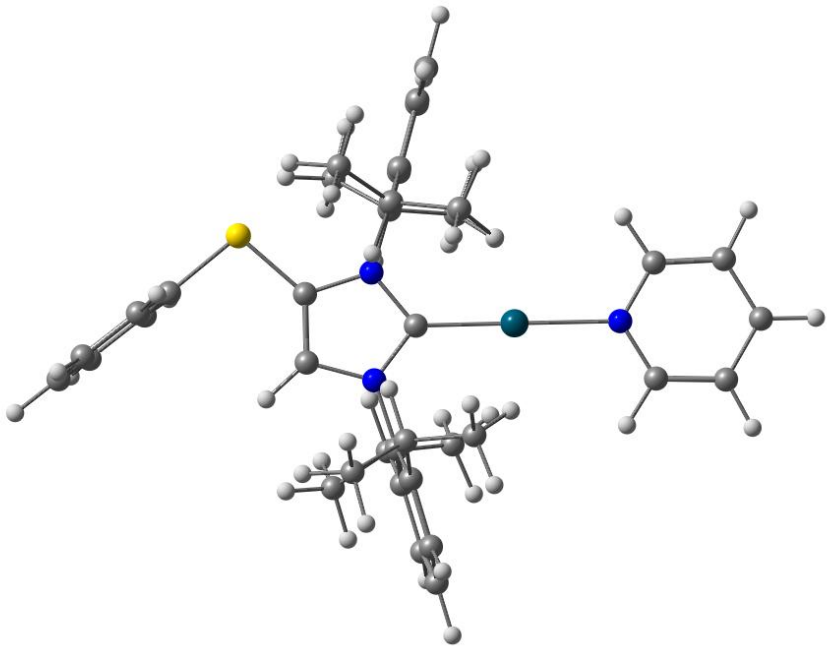
H	-2.8463640	-4.2090810	-2.2958200
H	-3.8682210	-3.1538180	-3.2994210
H	-1.5918250	-1.1606750	-4.1449400
H	-3.1760370	-0.6041460	-3.5557100
H	-1.6853590	-0.0511480	-2.7530200
H	1.4251580	-0.5212090	-4.0301810
H	1.3047060	0.3928910	-2.5035020
H	2.8189610	0.4197590	-3.4436540
H	2.7761450	-2.6931860	-4.1032030
H	4.2361700	-1.8223980	-3.5992510
H	3.6794310	-3.2331510	-2.6650680
H	-2.3268550	-1.7955860	4.8048450
H	-3.8990770	-1.3389490	4.1290010
H	-3.1598840	-2.8937870	3.6770220
H	-1.3545260	0.4173170	3.9646520
H	-1.3484300	0.7690900	2.2157700
H	-2.8670750	0.8818530	3.1450640
H	2.7505510	-1.8345770	4.6359010
H	3.4460920	-2.7204500	3.2536030
H	4.2764060	-1.2873430	3.9101020
H	1.6787020	0.4571550	4.2786270
H	3.1614580	1.0915080	3.5299410
H	1.6174350	1.1672340	2.6451290
S	2.3208340	-4.1958550	0.5599770
C	1.3976370	-5.7117010	0.7395820
C	1.0321730	-6.1582100	2.0133830
C	1.0873570	-6.4730050	-0.3914520
C	0.3436110	-7.3626880	2.1509040
C	0.3996650	-7.6771770	-0.2458290
C	0.0271530	-8.1212500	1.0232950
H	1.2888930	-5.5596740	2.8903250
H	1.3866080	-6.1180760	-1.3801940
H	0.0572340	-7.7121920	3.1457450
H	0.1572280	-8.2725950	-1.1293170
H	-0.5097420	-9.0663700	1.1348890

Coordinates of the optimized structure of **9b**



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9b E=-2164.01204195

Pd	0.0372910	1.0433840	-0.0847800
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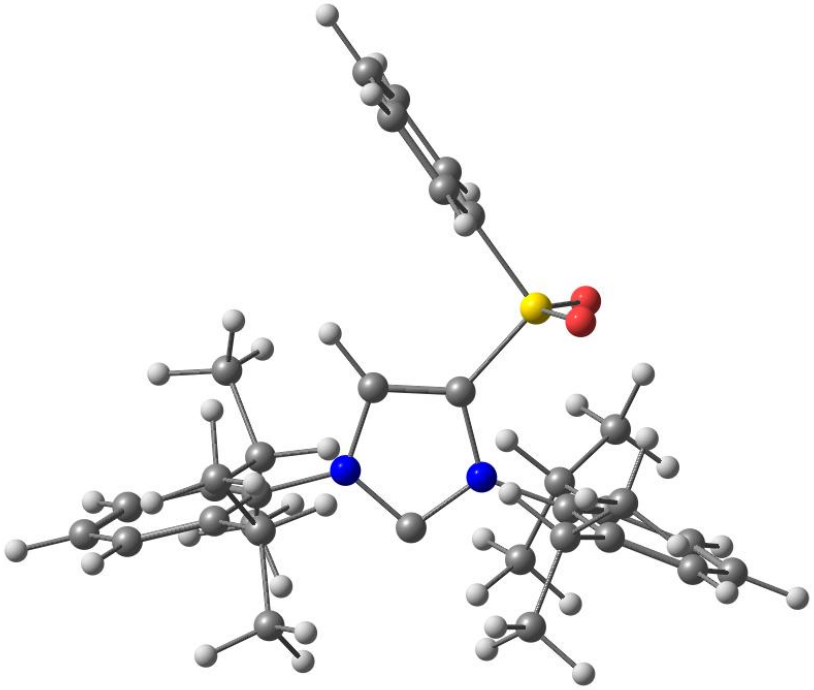
C	0.9838230	3.8939280	-0.4251700
C	-1.3123160	3.7256690	-0.3910370
C	0.9255560	5.2731530	-0.5962920
C	-1.4606600	5.0982030	-0.5606130
C	-0.3205730	5.8915690	-0.6660550
H	1.9418720	3.3731090	-0.3656900
H	-2.1820180	3.0705370	-0.3051880
H	1.8508280	5.8471400	-0.6731260
H	-2.4614980	5.5312390	-0.6084910
H	-0.4018140	6.9729190	-0.8001900
C	0.9963060	-3.0177090	0.4019470
C	-0.3608750	-3.1109730	0.3993750
N	1.3012230	-1.6737190	0.2389970
N	-0.8364780	-1.8169210	0.2389030
C	0.1696800	-0.9002710	0.1358810
C	2.6388160	-1.1710150	0.1766150
C	-2.2307540	-1.5036810	0.1927430
C	-2.9161940	-1.2818510	1.4019980
C	-4.2868960	-1.0106800	1.3336920
C	-4.9499880	-0.9656920	0.1114710
C	-4.2503150	-1.1917520	-1.0695280
C	-2.8788920	-1.4669490	-1.0559200
C	-2.1395810	-1.6996780	-2.3598260
C	-2.2113520	-1.2980940	2.7459110
C	3.2698330	-0.7674570	1.3687220
C	4.5826110	-0.2936530	1.2800610
C	5.2415810	-0.2279170	0.0565910
C	4.5982740	-0.6394260	-1.1061970
C	3.2860450	-1.1221920	-1.0728400
C	2.5989080	-1.5434150	-2.3585130
C	2.5703690	-0.8205860	2.7135100

H	-4.8445030	-0.8282080	2.2559600
H	-4.7798870	-1.1519820	-2.0249460
H	-1.0860420	-1.8952170	-2.1112620
C	-2.6743350	-2.9257710	-3.1016740
C	-2.1660620	-0.4476860	-3.2373950
H	-1.1670560	-1.5954450	2.5686850
H	5.0975060	0.0325080	2.1874100
H	5.1247130	-0.5826160	-2.0622060
H	1.6212120	-1.9696350	-2.0878450
C	2.3267980	-0.3308730	-3.2510920
C	3.3806970	-2.6308590	-3.0965350
H	1.5680600	-1.2432240	2.5475030
H	-1.0154380	-3.9709800	0.4987610
H	-6.0215120	-0.7522230	0.0791240
H	6.2674260	0.1464580	0.0090670
C	-2.8227260	-2.3236200	3.7012660
C	-2.1794380	0.1026660	3.3602170
C	3.3019470	-1.7381600	3.6946360
C	2.3727790	0.5842550	3.2846710
H	-2.0908360	-3.1057950	-4.0184160
H	-2.6143180	-3.8311430	-2.4780460
H	-3.7267700	-2.7932260	-3.4001910
H	-1.5739980	-0.6061870	-4.1527940
H	-3.1924160	-0.1877690	-3.5433970
H	-1.7367180	0.4095080	-2.6944980
H	1.7869710	-0.6355730	-4.1619790
H	1.7112620	0.4109460	-2.7171750
H	3.2647960	0.1564020	-3.5632780
H	2.8249940	-2.9621950	-3.9879060
H	4.3635020	-2.2685740	-3.4381960
H	3.5468030	-3.5074160	-2.4519760
H	-2.2549210	-2.3552200	4.6444970
H	-3.8661710	-2.0755820	3.9534850
H	-2.8140700	-3.3348330	3.2658250
H	-1.6212340	0.0953980	4.3100830
H	-1.6862900	0.8122750	2.6769990
H	-3.1956710	0.4736810	3.5705890
H	2.7429340	-1.8119960	4.6409410
H	3.4135230	-2.7525210	3.2818750
H	4.3078130	-1.3574180	3.9345950
H	1.8140550	0.5396410	4.2331390
H	3.3370160	1.0782560	3.4871510
H	1.8026880	1.2092370	2.5786790
S	2.2701140	-4.2167230	0.5656860
C	1.2685140	-5.6638540	0.8578010
C	0.8942580	-5.9985530	2.1631700
C	0.9017990	-6.4829440	-0.2141490
C	0.1399400	-7.1482900	2.3912880
C	0.1486840	-7.6327220	0.0222900
C	-0.2329440	-7.9644920	1.3224190
H	1.1960070	-5.3565940	2.9938510
H	1.2076810	-6.2157810	-1.2281300
H	-0.1535170	-7.4099950	3.4107220
H	-0.1386830	-8.2733710	-0.8148490
H	-0.8216140	-8.8668470	1.5046540

Coordinates of the optimized structure of **$PhSO_2$-IPr**



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PhSO2-IPr E=-1938.29326321

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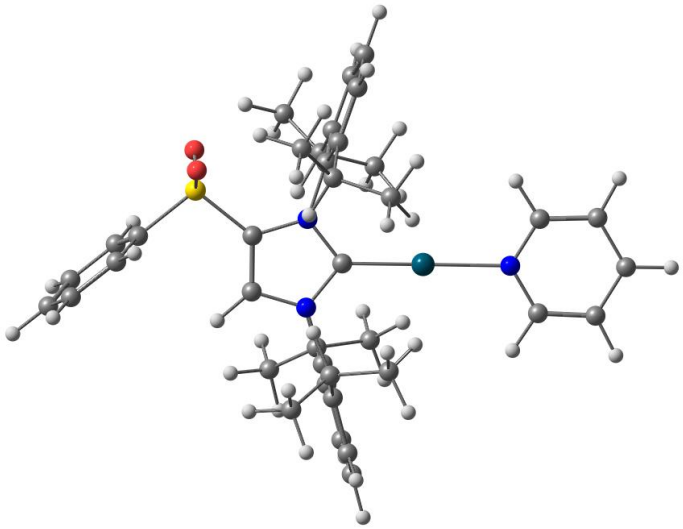
N	1.4637750	-1.6139170	0.1365000
N	-0.6325040	-1.9699310	0.2290110
C	0.2731940	-0.9593220	0.0628420
C	2.7368270	-0.9564980	0.0323530
C	-2.0523630	-1.7743690	0.2475240
C	-2.6909380	-1.5793760	1.4862300
C	-4.0804750	-1.4168350	1.4808980
C	-4.8018080	-1.4403920	0.2918850
C	-4.1442940	-1.6258570	-0.9197630
C	-2.7570880	-1.8002430	-0.9698740
C	-2.0613600	-1.9764680	-2.3066930
C	-1.9277330	-1.5391890	2.7981240
C	3.3370550	-0.4671940	1.2065830
C	4.5617790	0.1944020	1.0772050
C	5.1627710	0.3534540	-0.1675380
C	4.5504450	-0.1484540	-1.3108450
C	3.3240060	-0.8170770	-1.2373360
C	2.6396150	-1.3121170	-2.4977230
C	2.6654920	-0.5955830	2.5609330
H	-4.6066660	-1.2647380	2.4265480
H	-4.7198020	-1.6341050	-1.8487600
H	-1.0020220	-2.1953730	-2.1062240
C	-2.6278300	-3.1543800	-3.1003040
C	-2.1071730	-0.6774990	-3.1145460
H	-0.8552020	-1.6076950	2.5630750
H	5.0544010	0.5921640	1.9669420
H	5.0335370	-0.0176990	-2.2816920
H	1.8691390	-2.0361030	-2.1917860
C	1.9309610	-0.1518230	-3.2019180
C	3.5908760	-2.0481260	-3.4387120

H	1.9253820	-1.4069100	2.4842250
H	-0.6053730	-4.1216840	0.5454250
H	-5.8866030	-1.3089370	0.3092670
H	6.1210310	0.8731570	-0.2467540
C	-2.2816180	-2.7343860	3.6855980
C	-2.1391190	-0.2133650	3.5306610
C	3.6361940	-0.9879720	3.6719790
C	1.9060410	0.6909100	2.8963700
H	-2.0592040	-3.2954940	-4.0326430
H	-2.5742340	-4.0913440	-2.5248360
H	-3.6808590	-2.9913280	-3.3795380
H	-1.5553430	-0.7908990	-4.0609900
H	-3.1436740	-0.3963380	-3.3613390
H	-1.6544900	0.1524350	-2.5517720
H	1.3891290	-0.5099180	-4.0919840
H	1.2081290	0.3357610	-2.5307020
H	2.6570560	0.6088490	-3.5317750
H	3.0304280	-2.4630840	-4.2911280
H	4.3623410	-1.3804260	-3.8539920
H	4.0894230	-2.8781770	-2.9181400
H	-1.6904290	-2.7140180	4.6146250
H	-3.3466430	-2.7244360	3.9678870
H	-2.0797430	-3.6892140	3.1760190
H	-1.5215990	-0.1771570	4.4417970
H	-1.8592640	0.6402980	2.8955800
H	-3.1887490	-0.0791370	3.8368310
H	3.0846170	-1.1608860	4.6093930
H	4.1722170	-1.9122160	3.4125420
H	4.3768470	-0.1984340	3.8755480
H	1.3735930	0.5897850	3.8558060
H	2.5976550	1.5448210	2.9814520
H	1.1678110	0.9251090	2.1147090
S	2.6314020	-4.1303860	0.4891270
O	3.2949700	-4.2357790	-0.8108090
O	3.4167100	-3.7705260	1.6701490
C	1.7828700	-5.6564400	0.8173530
C	1.5064110	-6.0027470	2.1401470
C	1.4373130	-6.4807430	-0.2532230
C	0.8472470	-7.2038270	2.3909690
C	0.7786820	-7.6790970	0.0137190
C	0.4826810	-8.0358370	1.3305020
H	1.8152400	-5.3424890	2.9529670
H	1.6930590	-6.1848150	-1.2725350
H	0.6231540	-7.4952070	3.4194810
H	0.5009410	-8.3404800	-0.8098950
H	-0.0326270	-8.9776150	1.5336070

Coordinates of the optimized structure of **9c**



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9c E=-2314.3487229

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C	0.7886380	3.9112520	-0.4650010
C	-1.4871910	3.5908870	-0.3214950
C	0.6300900	5.2808330	-0.6487020
C	-1.7352220	4.9479930	-0.4992400
C	-0.6568170	5.8134280	-0.6671320
H	1.7813910	3.4562450	-0.4452120
H	-2.3064350	2.8811320	-0.1876620
H	1.5100190	5.9141250	-0.7752280
H	-2.7639440	5.3128500	-0.5050050
H	-0.8166020	6.8848840	-0.8097590
C	1.3344630	-2.9653560	0.3506230
C	-0.0116530	-3.1547530	0.3850610
N	1.5519250	-1.6030850	0.1976630
N	-0.5776740	-1.9098210	0.2546490
C	0.3658690	-0.9158390	0.1371280
C	2.8438250	-0.9800780	0.1242600
C	-1.9930740	-1.6907500	0.2475560
C	-2.6488950	-1.4642630	1.4714790
C	-4.0364530	-1.2894990	1.4402270
C	-4.7401950	-1.3395890	0.2414240
C	-4.0661620	-1.5647180	-0.9545870
C	-2.6797400	-1.7479420	-0.9792520
C	-1.9632290	-1.9515120	-2.3008540
C	-1.9042690	-1.3789990	2.7912320
C	3.4476620	-0.5377380	1.3165580
C	4.6930710	0.0892840	1.2150250
C	5.3135700	0.2602180	-0.0180910
C	4.6995110	-0.1975520	-1.1786930
C	3.4521740	-0.8289980	-1.1359260
C	2.7800040	-1.2699450	-2.4232470
C	2.7790730	-0.6820880	2.6715930
H	-4.5749720	-1.1078940	2.3737220
H	-4.6277340	-1.5959170	-1.8916230
H	-0.9113180	-2.1859090	-2.0787770
C	-2.5336230	-3.1260280	-3.0959280

C	-1.9686840	-0.6549590	-3.1134450
H	-0.8406620	-1.5741280	2.5882440
H	5.1862770	0.4505070	2.1203030
H	5.1970720	-0.0593270	-2.1413980
H	1.9394920	-1.9258230	-2.1494220
C	2.1986640	-0.0600880	-3.1593940
C	3.7094690	-2.0832020	-3.3227360
H	1.9390220	-1.3836660	2.5527190
H	-0.5980730	-4.0628210	0.4914100
H	-5.8242660	-1.2005140	0.2388810
H	6.2880400	0.7521860	-0.0745930
C	-2.3832110	-2.4383080	3.7850390
C	-1.9937030	0.0314390	3.3768500
C	3.7150860	-1.2758290	3.7239920
C	2.1964200	0.6578890	3.1281930
H	-1.9503650	-3.2824560	-4.0167390
H	-2.5057150	-4.0600350	-2.5135040
H	-3.5785490	-2.9487320	-3.3962350
H	-1.3978900	-0.7805370	-4.0473020
H	-2.9947930	-0.3551890	-3.3818240
H	-1.5078270	0.1604650	-2.5317540
H	1.6564550	-0.3808540	-4.0636010
H	1.4987380	0.4923210	-2.5096060
H	2.9978980	0.6315540	-3.4728140
H	3.1573640	-2.4454040	-4.2043840
H	4.5527930	-1.4799580	-3.6948400
H	4.1094460	-2.9539180	-2.7847640
H	-1.7920040	-2.3885330	4.7128760
H	-3.4402130	-2.2912820	4.0590820
H	-2.2824430	-3.4540780	3.3721720
H	-1.4036070	0.1013680	4.3043900
H	-1.5998560	0.7712590	2.6617500
H	-3.0338780	0.3024690	3.6194970
H	3.1666630	-1.4432930	4.6645290
H	4.1240630	-2.2380090	3.3853500
H	4.5539010	-0.6001830	3.9550050
H	1.6691940	0.5426780	4.0891420
H	2.9931210	1.4069300	3.2683190
H	1.4814870	1.0468810	2.3827090
S	2.6154360	-4.1809300	0.4513340
O	3.2566090	-4.2932780	-0.8590560
O	3.4358430	-3.8941720	1.6278780
C	1.6910170	-5.6674640	0.7548100
C	1.4085430	-6.0284930	2.0723710
C	1.2937180	-6.4481860	-0.3302880
C	0.6907570	-7.1994910	2.3032310
C	0.5768390	-7.6171190	-0.0832310
C	0.2748680	-7.9877970	1.2282980
H	1.7568280	-5.4021550	2.8960140
H	1.5545750	-6.1417650	-1.3451950
H	0.4604530	-7.5018090	3.3272060
H	0.2575730	-8.2444760	-0.9183390
H	-0.2864080	-8.9062530	1.4158120

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